

Figure S1. A. Distribution of basic amines and carboxylic acids in the CNS and non-CNS oral drugs. Clearly majority of the CNS drugs had a basic amine and only 30% of non-CNS oral drugs had the basic amine. Carboxylic acids were not favored for either of the drug classes. It was especially not favored for CNS drugs.

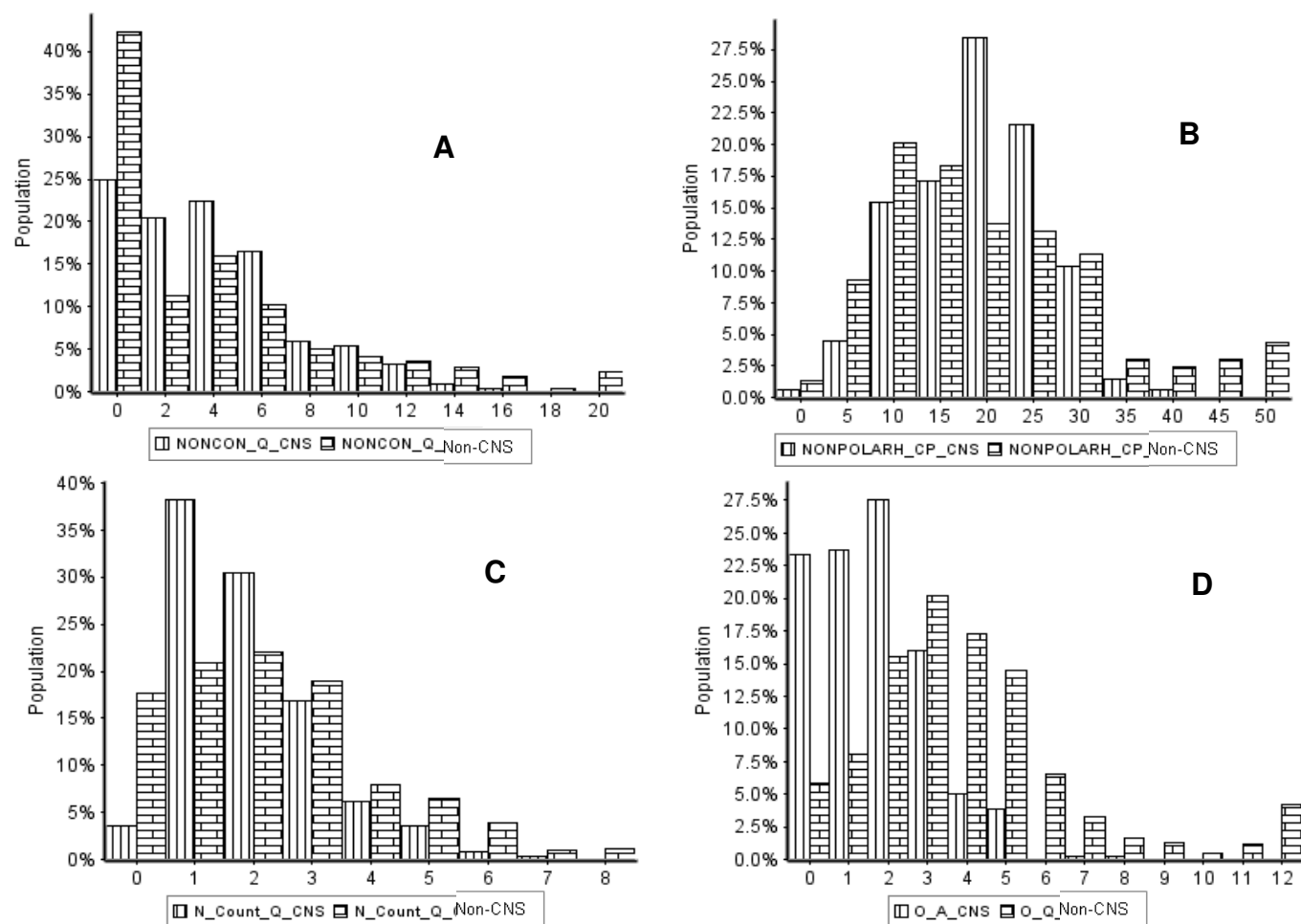


Figure S2. A. Distribution of non-conjugated atoms (number of ring atoms not able to form conjugated aromatic systems); B. Nonpolar hydrogen atoms(best range 20-24); C. Number of nitrogen atoms (best range 1-2); D. Number of oxygen atoms (best range 0-2).

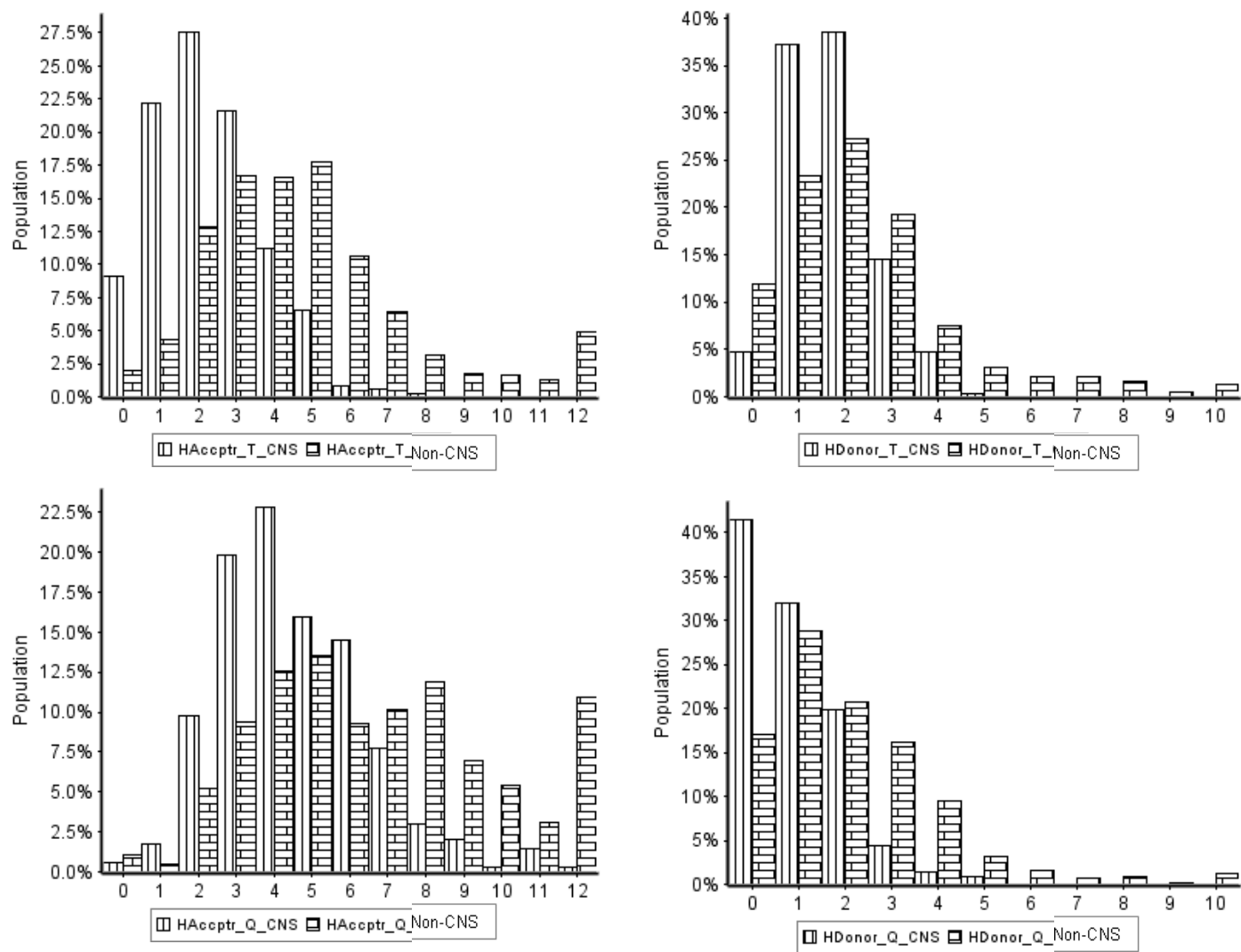


Figure S3. A. Distribution of hydrogen bond acceptors and donors, as computed by Tripos and QikProp (Schrodinger) software.

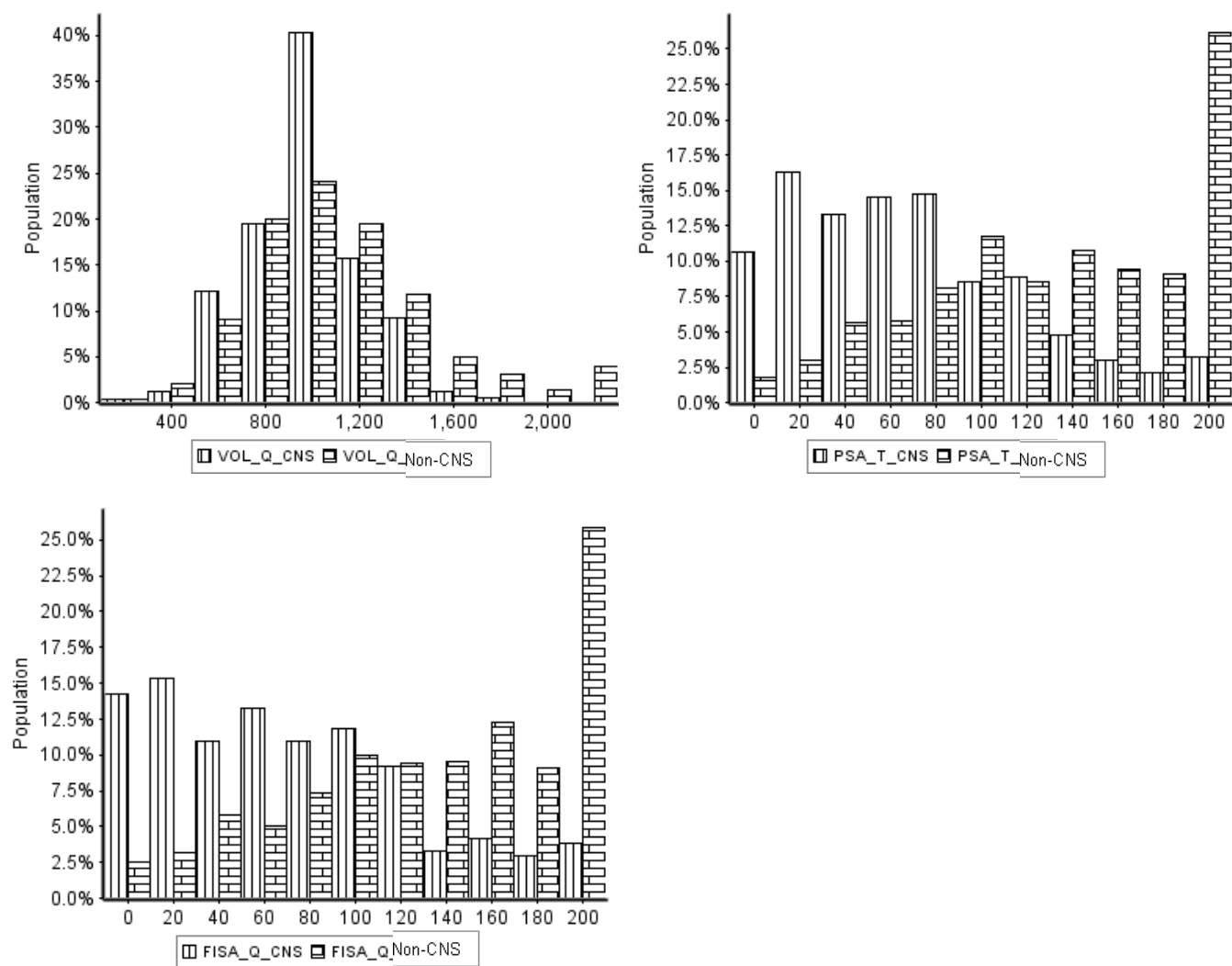


Figure S4. A. Distribution of molecular volume, hydrophobic surface area as computed by QP and polar surface area (solvent accessible) as computed by Tripos.

Table S1. CNS drug set with the indication and the mechanism of action.

Number	SMILES	GENERIC_NAME	Indication	Mechanism
1	<chem>CC(=O)Nc1nnc(s1)S(=O)(=O)N</chem>	ACETAZOLAMIDE	Anticonvulsants	inhibition of carbonic anhydrase in the CNS
2	<chem>CC(=O)c1ccc2c(c1)N(c3ccccc3S2)CCCN4CCN(CC4)CCO</chem>	ACETOPHENAZINE	Antipsychotics	blocks postsynaptic mesolimbic dopaminergic D1 and D2 receptors in the brain
3	<chem>CCC(=O)N(c1ccccc1)C2(CCN(CC2)CCn3c(=O)n(nn3)CC)COC</chem>	ALFENTANIL	For the management of postoperative pain and the maintenance of general anesthesia.	interacts predominately with the opioid mu-receptor. In clinical settings, alfentanil exerts its principal pharmacologic effects on the central nervous system.
4	<chem>Cc1nnc2n1-c3ccc(cc3C(=NC2)c4ccccc4)Cl</chem>	ALPRAZOLAM	management of anxiety disorder	benzodiazepine receptors BNZ1, which mediates sleep, and BNZ2, which affects muscle relaxation, anticonvulsant activity, motor coordination, and memory.

5	<chem>C1C2CC3CC1CC(C2)(C3)N</chem>	AMANTADINE	treatment of parkinsonism	The mechanism of its antiparkinsonic effect is not fully understood, but it appears to be releasing dopamine from the nerve endings of the brain cells, together with stimulation of norepinephrine response.
6	<chem>Cn1c2c(c(=O)n(c1=O)C)[nH]cn2</chem>	AMINOPHYLLINE	treatment of bronchospasm due to asthma	Aminophylline is the ethylenediamine salt of theophylline. Theophylline stimulates the CNS, skeletal muscles, and cardiac muscle
7	<chem>CCN1CCCC1CNC(=O)c2cc(c(cc2OC)N)S(=O)(=O)CC</chem>	AMISULPRIDE	Antipsychotic Agents	Amisulpride binds selectively to dopamine D(2) and D(3) receptors in the limbic system.
8	<chem>CN(C)CCC=C1c2ccccc2CCc3c1cccc3</chem>	AMITRIPTYLINE	treatment of anxiety, bipolar disorders, and depression	Amitriptyline is metabolized to nortriptyline which inhibits the reuptake of norepinephrine and serotonin almost equally.
9	<chem>CC(Cc1ccccc1)N</chem>	AMPHETAMINE	treatment of Attention Deficit Disorder with Hyperactivity (ADDH) and narcolepsy in children	Amphetamines stimulate the release of norepinephrine from central adrenergic receptors.

10	<chem>CCC1(C(=O)NC(=O)NC1=O)CCC(C)C</chem>	AMOBARBITAL	Amnesia, Insomnia, Epilepsy	Amobarbital (like all barbiturates) works by binding to the GABAA receptor at either the alpha or the beta sub unit.
11	<chem>COc1ccc(cc1)C(=O)N2CCCC2=O</chem>	ANIRACETAM	cognitive enhancer, Antidepressant	NOT APPROVED
12	<chem>CN1CCc2cccc-3c2C1Cc4c3c(c(cc4)O)O</chem>	APOMORPHINE	Antiparkinson Agent	it is believed to be due to stimulation of post-synaptic dopamine D2-type receptors within the brain
13	<chem>Cc1cccc1OC(CCNC)c2cccc2</chem>	ATOMOXETINE	treatment of attention-deficit hyperactivity disorder (ADHD).	Mechanism of action is unknown, but is thought to be related to selective inhibition of the pre-synaptic norepinephrine transporter,
14	<chem>CN1CCC(=C2c3ccccc3CCc4c2nccc4)CC1</chem>	AZATADINE	For the relief of the symptoms of upper respiratory mucosal congestion in perennial and allergic rhinitis, and for the relief of nasal congestion and eustachian t.b. congestion	Azatadine is an antihistamine, related to cyproheptadine, with anti-serotonin, anticholinergic (drying), and sedative effects.

15	<chem>c1cc(ccc1C(CC(=O)O)CN)Cl</chem>	BACLOFEN	For the alleviation of signs and symptoms of spasticity resulting from multiple sclerosis, particularly for the relief of flexor spasms and concomitant pain, clonus, and muscular rigidity.	Baclofen is a direct agonist at GABAB receptors. The precise mechanism of action of Baclofen is not fully known. It is capable of inhibiting both monosynaptic and polysynaptic reflexes at the spinal level, possibly by hyperpolarization of afferent terminals,
16	<chem>c1ccc2c(c1)[nH]c(=O)n2C3CCN(CC3)CCCC(=O)c4ccc(cc4)F</chem>	BENPERIDOL	Antipsychotic which can be used for the treatment of schizophrenia.	Pretreatment of an animal with unlabeled receptor-specific antagonists prior to injection of [18F]BP confirmed that the radioligand bound specifically to central D2 receptors in vivo
17	<chem>c1ccc(cc1)C(CCN2CCC2)(C3CCCCC3)O</chem>	BENZHEXOL	Antiparkinson Agents	Trihexyphenidyl partially blocks cholinergic activity in the CNS, which is responsible for the symptoms of Parkinson's disease.
18	<chem>CC(Cc1ccccc1)N(C)Cc2ccccc2</chem>	BENZPHETAMINE	Central Nervous System Stimulants, for the management of exogenous obesity as a short term adjunct (a few weeks) in a regimen of weight reduction based on caloric restriction	stimulate the release of norepinephrine and/or dopamine from storage sites in nerve terminals in the lateral hypothalamic feeding center, thereby producing a decrease in appetite. This release is mediated by the binding of benzphetamine to centrally located adrenergic receptors.
19	<chem>CN1C2CCC1CC(C2)OC(c3ccccc3)c4ccccc4</chem>	BENZTROPINE	For use as an adjunct in the therapy of all forms of parkinsonism and also for use in the control of extrapyramidal disorders due to neuroleptic drugs.	Benztropine partially blocks cholinergic activity in the CNS, which is responsible for the symptoms of Parkinson's disease. I

20	<chem>CNCCc1cccn1</chem>	BETAHISTINE	For the reduction of episodes of vertigo associated with Ménière's disease	H3-receptor antagonism increases the levels of neurotransmitters such as serotonin in the brainstem, which inhibits the activity of vestibular nuclei, helping to restore proper balance and decrease in vertigo symptoms.
21	<chem>c1ccc(cc1)C(CCN2CC(CCC2)(C3CC4CC3C=C4)O</chem>	BIPERIDEN	For use as an adjunct in the therapy of all forms of parkinsonism and control of extrapyramidal disorders secondary to neuroleptic drug therapy	The mechanism of action of centrally active anticholinergic drugs such as biperiden is considered to relate to competitive antagonism of acetylcholine at cholinergic receptors in the corpus striatum, which then restores the balance.
22	<chem>c1ccnc(c1)C2=NCC(=O)Nc3c2cc(cc3)Br</chem>	BROMAZEPAM	For the short-term treatment of insomnia, short-term treatment of anxiety or panic attacks	Bromazepam binds to the GABA receptor GABAA, causing a conformational change and increasing inhibitory effects of GABA. Other neurotransmitters are not influenced
23	<chem>CC(C)CC1C(=O)N2CC(C2C3(N1C(=O)C(O3)(C(C)C)NC(=O)C4CN(C5Cc6c7c(ccc7[nH]c6Br)C5=C4)C)O</chem>	BROMOCRIPTINE	as monotherapy in early Parkinsonian Syndrome	Bromocriptine stimulates centrally-located dopaminergic receptors resulting in a number of pharmacologic effects.
24	<chem>CN(C)CCC(c1ccc(cc1)Br)c2cccn2</chem>	BROMPHENIRAMINE	For the treatment of the symptoms of the common cold and allergic rhinitis, such as runny nose, itchy eyes, watery eyes, and sneezing	Brompheniramine works by acting as an antagonist of the H1 histamine receptors. Its effects on the cholinergic system may include side-effects such as drowsiness, sedation, dry mouth, dry throat, blurred vision, and increased heart rate.

25	<chem>Cc1nnc2n1-c3c(cc(s3)Br)C(=NC2)c4ccccc4Cl</chem>	BROTIZOLAM	Brotizolam is prescribed for the short term treatment, 2 - 4 weeks only of moderately severe insomnia	Brotizolam has been shown in animal studies to be a very high potency benzodiazepine
26	<chem>CC(C)(C)C(C)(C1CC23CCC1(C4C25CCN(C3Cc6c5c(c(cc6)O)O4)C7CC7)OC)O</chem>	BUPRENORPHINE	For the treatment of moderate to severe pain, peri-operative analgesia, and opioid dependence.	Buprenorphine's analgesic effect is due to partial agonist activity at mu-opioid receptors. Buprenorphine is also a kappa-opioid receptor antagonist.
27	<chem>CC(C(=O)c1cccc(c1)Cl)NC(C)(C)C</chem>	BUPROPION	For the treatment of depression and as aid to smoking cessation.	Bupropion selectively inhibits the neuronal reuptake of dopamine, norepinephrine, and serotonin;
28	<chem>c1cnc(nc1)N2CCN(CC2)CCCCN3C(=O)CC4(CCCC4)CC3=O</chem>	BUSPIRONE	For the management of anxiety disorders or the short-term relief of the symptoms of anxiety, and also as an augmentation of SSRI-treatment against depression	Buspirone binds to 5-HT type 1A serotonin receptors on presynaptic neurons in the dorsal raphe and on postsynaptic neurons in the hippocampus, thus inhibiting the firing rate of 5-HT-containing neurons in the dorsal raphe.
29	<chem>CC(C)CC1(C(=O)NC(=O)NC1=O)CC=C</chem>	BUTALBITAL	Used in combination with acetaminophen or aspirin and caffeine for its sedative and relaxant effects in the treatment of tension headaches, migraines, and pain	Butalbital binds at a distinct binding site associated with a Cl ⁻ ionopore at the GABAA receptor, increasing the duration of time for which the Cl ⁻ ionopore is open. The post-synaptic inhibitory effect of GABA in the thalamus is, therefore, prolonged.

30	<chem>CCC(C)C1(C(=O)NC(=O)NC1=O)CC</chem>	BUTOBARBITONE	For the treatment of insomnia	Butethal binds at a distinct binding site associated with a Cl ⁻ ionophore at the GABAA receptor, increasing the duration of time for which the Cl ⁻ ionophore is open
31	<chem>CCCCC(CC)CNC(=O)CC(C)O</chem>	BUTOCTAMIDE HYDROGEN SUCCINATE	For the treatment of insomnia	Unlike other hypnotics, butocamide appears to increase REM sleep.
32	<chem>c1cc2c(cc1O)C34CCC(CC3(C(C2)N(CC4)CC5CCC5)O</chem>	BUTORPHANOL	For the relief of moderate to severe pain	The exact mechanism of action is unknown, but is believed to interact with an opiate receptor site in the CNS (probably in or associated with the limbic system).
33	<chem>CCNC(=O)N(CCCN(C)C)C(=O)C1CC2c3cccc4c3c(c[nH]4)CC2N(C1)CC=C</chem>	CABERGOLINE	May also be used to manage symptoms of Parkinsonian Syndrome as monotherapy during initial symptomatic management or as an adjunct to levodopa therapy during advanced stages of disease	Cabergoline stimulates centrally-located dopaminergic receptors resulting in a number of pharmacologic effects.
34	<chem>Cn1cnc2c1c(=O)n(c(=O)n2C)C</chem>	CAFFEINE	For management of fatigue, orthostatic hypotension, and for the short term treatment of apnea of prematurity in infants.	Caffeine, a naturally occurring xanthine derivative like theobromine and the bronchodilator theophylline, is used as a CNS stimulant, mild diuretic, and respiratory stimulant (in neonates with apnea of prematurity).

35	<chem>c1ccc2c(c1)C=Cc3cccc3N2C(=O)N</chem>	CARBAMAZEPINE	For the treatment of epilepsy and pain associated with true trigeminal neuralgia	Carbamazepine also possesses anticholinergic, central antidiuretic, antiarrhythmic, muscle relaxant, antidepressant (possibly through blockade of norepinephrine release), sedative, and neuromuscular-blocking properties.
36	<chem>c1ccc2c(c1)CCc3cccc3N2CCCN4CCC(CC4)C(=O)N)N5CCCCC5</chem>	CARPIPRAMINE	an atypical antipsychotic used for the treatment of schizophrenia and anxiety in France and Japan	potent DA antagonists which block α 1- and α 2-adrenoceptors in the brain. European Journal of Pharmacology, Volume 112, Issue 3, 19 June 1985, Pages 313-322
37	<chem>Cc1c(scnc1)CCCI</chem>	CHLOMETHIAZOLE	a sedative and hypnotic that is widely used in treating and preventing symptoms of acute alcohol withdrawal.	Chlomethiazole acts as a positive allosteric modulator at the barbiturate/picrotoxin site of the GABA-A receptor. It works to enhance the action of the neurotransmitter GABA at this receptor. GABA is the major inhibitory neurotransmitter in the brain and produces anxiolytic, anticonvulsant, sedative, and hypnotic effects.
38	<chem>C(C(Cl)(Cl)Cl)(O)O</chem>	CHLORAL HYDRATE	Chloral hydrate is used for the short-term treatment of insomnia and as a sedative before minor medical or dental treatment	Chloral hydrate exerts its pharmacological properties via enhancing the GABA receptor complex
39	<chem>c1ccc(cc1)C2=NC(C(=O)Nc3c2cc(cc3)Cl)C(=O)O</chem>	CHLORAZEPATE	For the management of anxiety disorders or for the short-term relief of the symptoms of anxiety.	Benzodiazepines bind nonspecifically to benzodiazepine receptors BNZ1, which mediates sleep, and BNZ2, which affects muscle relaxation, anticonvulsant activity, motor coordination, and memory.

40	<chem>C/N=C\1/CN(C(=c2cc(c2=N1)Cl)c3ccccc3)O</chem>	CHLORDIAZEPOXIDE	For the management of anxiety disorders or for the short-term relief of symptoms of anxiety, withdrawal symptoms of acute alcoholism, and preoperative apprehension and anxiety	Chlordiazepoxide binds to stereospecific benzodiazepine (BZD) binding sites on GABA (A) receptor complexes at several sites within the central nervous system, including the limbic system and reticular formation.
41	<chem>CN1C(S(=O)(=O)CCC1=O)c2ccc(cc2)Cl</chem>	CHLORMEZANONE	Used in the management of anxiety and in the treatment of muscle spasm	Chlormezanone binds to central benzodiazepine receptors which interact allosterically with GABA receptors.
42	<chem>c1cc(ccc1OCC(CO)O)Cl</chem>	CHLORPHENESIN	Used, along with rest and physical therapy, to treat injuries and other painful muscular conditions.	It is known that chlorphenesin acts in the central nervous system (CNS) rather than directly on skeletal muscle.
43	<chem>CN(C)CCC(c1ccc(cc1)Cl)c2cccn2</chem>	CHLORPHENIRAMINE	For the treatment of rhinitis, urticaria, allergy, common cold, asthma and hay fever.	In addition to being an histamine H1 receptor antagonist, chlorpheniramine has been shown to work as a serotonin-norepinephrine reuptake inhibitor or SNRI
44	<chem>CN(C)CCCN1c2ccccc2Sc3c1cc(cc3)Cl</chem>	CHLORPROMAZINE	For the treatment of schizophrenia, control nausea and vomiting.	Chlorpromazine acts as an antagonist (blocking agent) on different postsynaptic receptors (D1, D2, D3 and D4 ; 5-HT1 and 5-HT2; H1)

45	<chem>CN(C)CC/C=C\c2ccc(cc2Sc3c1cc(cc3)Cl</chem>	CHLORPROTHIXINE	For treatment of psychotic disorders (e.g. schizophrenia) and of acute mania occurring as part of bipolar disorders.	Chlorprothixene blocks postsynaptic mesolimbic dopaminergic D1 and D2 receptors in the brain;
46	<chem>c1cc2c(cc1Cl)[nH]c(=O)o2</chem>	CHLORZOXAZONE	For the relief of discomfort associated with acute painful musculoskeletal conditions	A centrally acting central muscle relaxant with sedative properties. It is claimed to inhibit muscle spasm by exerting an effect primarily at the level of the spinal cord and subcortical areas of the brain.
47	<chem>c1ccc(cc1)/C=C/CN2C(CN(CC2)C(c3ccccc3)c4ccccc4</chem>	CINNARIZINE	For the treatment of vertigo/meniere's disease, nausea and vomiting, motion sickness and also useful for vestibular symptoms of other origins.	Cinnarizine could be also viewed as a nootropic drug because of its vasorelaxating abilities (due to calcium channel blockage), which happen mostly in brain. It is also effectively combined with other nootropics, primarily piracetam; in such combination each drug potentiate the other in boosting brain oxygen supply.
48	<chem>c1ccc(c(c1)C2=NC(C(=O)N(c3c2cc(cc3)Cl)CC(C#N)O)F</chem>	CINOLAZEPAM	For the management of anxiety disorders or for the short-term relief of the symptoms of anxiety or anxiety associated with depressive symptoms.	Cinolazepam binds to central benzodiazepine receptors which interact allosterically with GABA receptors.
49	<chem>CN(C)CCCC1(c2ccc(cc2CO1)C#N)c3ccc(cc3)F</chem>	CITALOPRAM/ES CITALOPRAM	For the treatment of depression	The antidepressant, antiobsessive-compulsive, and anti bulimic actions of Citalopram are presumed to be linked to its inhibition of CNS neuronal uptake of serotonin.

50	<chem>CC(c1ccccc1)(c2ccc(cc2)Cl)OCCCN3CCCN3C</chem>	CLEMASTINE	For the relief of symptoms associated with allergic rhinitis such as sneezing, rhinorrhea, pruritus and acrimation.	Clemastine is an antihistamine with anticholinergic (drying) and sedative side effects.
51	<chem>CN1c2ccc(cc2N(C(=O)CC1=O)c3ccccc3)Cl</chem>	CLOBAZAM	For treatment and management of epilepsy and anxiety disorder.	Clobazam binds at a distinct binding site associated with a Cl ⁻ ionopore at the GABA-A receptor, increasing the duration of time for which the Cl ⁻ ionopore is open.
52	<chem>CN(C)CCCN1c2ccccc2CCc3c1cc(cc3)Cl</chem>	CLOMIPRAMINE	For the treatment of depression, obsessive compulsive disorder (OCD), panic attacks with or without agoraphobia, narcolepsy, chronic pain, and enuresis	Clomipramine, a tricyclic antidepressant, is the 3-chloro derivative of Imipramine. It is now thought that changes occur in receptor sensitivity in the cerebral cortex and hippocampus.
53	<chem>c1ccc(c(c1)C2=NCC(=O)Nc3c2cc(cc3)[N+](=O)[O-])Cl</chem>	CLONAZEPAM	Used as an anticonvulsant in the treatment of the Lennox-Gastaut syndrome (petit mal variant), akinetic and myoclonic seizures.	Allosteric interactions between central benzodiazepine receptors and gamma-aminobutyric acid (GABA) receptors potentiate the effects of GABA.
54	<chem>c1cc(c(c(c1)Cl)NC2=NCN2)Cl</chem>	CLONIDINE	May be used as an adjunct in the treatment of hypertension	Clonidine, a hypotensive agent, is a centrally-acting α_2 -adrenergic agonist. It crosses the blood-brain barrier and acts in the hypothalamus to induce a decrease in blood pressure. It

55	<chem>CN1CCN(CC1)C2=Nc3cc(ccc3Nc4c2cccc4)Cl</chem>	CLOZAPINE	For use in patients with treatment-resistant schizophrenia	Clozapine's antipsychotic action is likely mediated through a combination of antagonistic effects at D2 receptors in the mesolimbic pathway and 5-HT2A receptors in the frontal cortex.
56	<chem>CN1C2CCC1C(C(C2)OC(=O)c3ccccc3)C(=O)OC</chem>	COCAINE	For the introduction of local (topical) anesthesia of accessible mucous membranes of the oral, laryngeal and nasal cavities.	Cocaine produces anesthesia by inhibiting excitation of nerve endings or by blocking conduction in peripheral nerves. Cocaine, like amphetamines, acts by multiple mechanisms on brain catecholaminergic neurons; the mechanism of its reinforcing effects is thought to involve inhibition of dopamine uptake.
57	<chem>CN1CCC23c4c5ccc(c4OC2C(C=CC3C1C5)O)OC</chem>	CODEINE	For treatment and management of pain (Systemic), also used as an Antidiarrheal and as a cough suppressant	Codeine, an opiate agonist in the CNS, is similar to other phenanthrene derivatives such as morphine.
58	<chem>CN1CCN(CC1)C(c2ccc(cc2)c3ccccc3</chem>	CYCLIZINE	For prevention and treatment of nausea, vomiting, and dizziness associated with motion sickness, and vertigo	Although the mechanism by which cyclizine exerts its antiemetic and antivertigo effects has not been fully elucidated, its central anticholinergic properties are partially responsible.
59	<chem>CN(C)CCC=C1c2ccccc2C=Cc3c1cccc3</chem>	CYCLOBENZAPRINE	For use as an adjunct to rest and physical therapy for relief of muscle spasm associated with acute, painful musculoskeletal conditions.	Cyclobenzaprine is a skeletal muscle relaxant and a central nervous system (CNS) depressant. Cyclobenzaprine acts on the locus coeruleus where it results in increased norepinephrine release, potentially through the gamma fibers which innervate and inhibit the alpha motor neurons in the ventral horn of the spinal cord.

60	<chem>CN1CCC(=C2c3ccccc3C=Cc4c2cccc4)CC1</chem>	CYPROHEPTADINE	For treatment of perennial and seasonal allergic rhinitis, vasomotor rhinitis, allergic conjunctivitis due to inhalant allergens and foods, mild uncomplicated allergic skin manifestations of urticaria and angioedema, amelioration of allergic reactions to blood or plasma, cold urticaria, dermatographism, and as therapy for anaphylactic reactions adjunctive to epinephrine.	Cyproheptadine is a piperidine antihistamine. Unlike other antihistamines, this drug also antagonizes serotonin receptors. This action makes Cyproheptadine useful in conditions such as vascular headache and anorexia.
61	<chem>CCOC(=O)C1(CCN(C1)C)c2ccccc2</chem>	MEPERIDINE	Used to control moderate to severe pain.	Meperidine is primarily a kappa-opiate receptor agonist and also has local anesthetic effects. Meperidine has more affinity for the kappa-receptor than morphine.
62	<chem>C(C(F)(F)F)(OC(F)F)F</chem>	DESFLURANE	For use as an inhalation agent for induction and/or maintenance of anesthesia for inpatient and outpatient surgery in adults.	Desflurane induces a reduction in junctional conductance by decreasing gap junction channel opening times and increasing gap junction channel closing times. Desflurane also binds to and agonizes the GABA receptor, the large conductance Ca ²⁺ activated potassium channel, the glycine receptors, and antagonizes the glutamate receptors.
63	<chem>CNCCCN1c2ccccc2CCc3c1cccc3</chem>	DESIPRAMINE	For relief of symptoms in various depressive syndromes, especially endogenous depression.	The acute effects of desipramine include inhibition of noradrenaline re-uptake at noradrenergic nerve endings and inhibition of serotonin (5-hydroxy tryptamine, 5HT) re-uptake at the serotonergic nerve endings in the central nervous system.

64	<chem>CC1CC2C3CCC4=CC(=O)C=CC4(C3C(CC2C1C(=O)CO)O)C)O)F</chem>	DEXAMETHASONE	For the treatment of cerebral edema.	Used for its antiinflammatory or immunosuppressive properties and ability to penetrate the CNS, dexamethasone is used alone to manage cerebral edema and with tobramycin to treat corticosteroid-responsive inflammatory ocular conditions.
65	<chem>CCNC(C)Cc1cccc(c1)C(F)(F)F</chem>	FENFLURAMINE	For the management of exogenous obesity as a short-term (a few weeks) adjunct in a regimen of weight reduction based on caloric restriction.	Fenfluramine binds to the serotonin reuptake pump. This causes inhibition of serotonin uptake and release of serotonin. The increased levels of serotonin lead to greater serotonin receptor activation which in turn lead to enhancement of serotonergic transmission in the centres of feeding behavior located in the hypothalamus.
66	<chem>Cc1cccc(c1C)C(C)c2c[nH]cn2</chem>	DEXMEDETOMIDINE	For sedation of initially intubated and mechanically ventilated patients during treatment in an intensive care setting, also used in pain relief; anxiety reduction and analgesia	Dexmedetomidine activates 2-adrenoceptors, and causes the decrease of sympathetic tone, with attenuation of the neuroendocrine and hemodynamic responses to anesthesia and surgery; it reduces anesthetic and opioid requirements; and causes sedation and analgesia.
67	<chem>COC(=O)C(c1ccccc1)C2CCCN2</chem>	METHYLPHENIDATE	A central nervous system stimulant used most commonly in the treatment of attention-deficit disorders in children and for narcolepsy.	Methylphenidate blocks dopamine uptake in central adrenergic neurons by blocking dopamine transport or carrier proteins. Methylphenidate acts at the brain stem arousal system and the cerebral cortex and causes increased sympathomimetic activity in the central nervous system.

68	<chem>CC(CN1CCOCC1)C(c2ccccc2)(c3ccccc3)C(=O)N4CCCC4</chem>	DEXTROMORAMIDE	Dextromoramide is sometimes also used as a short-acting analgesic for minor surgical procedures. Another application that has been trialled in the Netherlands is prescription of oral dextromoramide as a way to try to reduce injecting drug use in recidivist opioid addicts who continued to abuse heroin despite being maintained on methadone.	Dextromoramide (Palfium, Palphium, Jetricum, Dimorlin) is a powerful opioid analgesic approximately three times more potent than morphine but shorter acting. It is subject to drug prohibition regimes.
69	<chem>CCC(=O)OC(Cc1ccccc1)(c2ccccc2)C(C)CN(C)C</chem>	DEXTROPROPOXYPHENE	For the relief of mild to moderate pain.	Propoxyphene acts as a weak agonist at OP1, OP2, and OP3 opiate receptors within the central nervous system
70	<chem>CC(=O)Oc1ccc2c3c1OC4C35CCN(C(C2)C5C=CC4OC(=O)C)C</chem>	DIAMORPHINE	Used in the treatment of acute pain, myocardial infarction, acute pulmonary oedema, and chronic pain.	Heroin is a mu-opioid agonist. It acts on endogenous mu-opioid receptors that are spread in discrete packets throughout the brain, spinal cord and gut in almost all mammals.
71	<chem>CN1c2ccc(cc2C(=NCC1=O)c3ccccc3)Cl</chem>	DIAZEPAM	Used in the treatment of severe anxiety disorders, as a hypnotic in the short-term management of insomnia, as a sedative and premedicant, as an anticonvulsant, and in the management of alcohol withdrawal syndrome.	Benzodiazepines bind nonspecifically to benzodiazepine receptors which mediate sleep, affects muscle relaxation, anticonvulsant activity, motor coordination, and memory.

72	<chem>CN1c2ccccc2C(=O)N(c3c1cccc3)CCN(C)C</chem>	NOVERIL	Antidepressive agent used in: Switzerland, Czech Republic, Hungary, Israel, Luxembourg, Poland, Slovakia Noveril is NOT known to be marketed in the USA.	It blocks the uptake of norepinephrine and serotonin into axon terminals and may block some subtypes of serotonin, adrenergic, and histamine receptors.
73	<chem>c1ccc(c(c1)CC(=O)O)Nc2c(cccc2Cl)Cl</chem>	DICLOFENAC	Diclofenac is an acetic acid nonsteroidal antiinflammatory drug (NSAID) with analgesic and antipyretic properties.	Antipyretic effects may be due to action on the hypothalamus, resulting in peripheral dilation, increased cutaneous blood flow, and subsequent heat dissipation.
74	<chem>CC(C)CC1C(=O)N2CC(C2C3(N1C(=O)C(O3)(C(C)C)NC(=O)C4CC5c6cccc7c6c(c[nH]7)CC5N(C4)C)O</chem>	ERGOLOID MESYLATE	For use as an adjunct therapy for patients with dementia	Ergoloid mesylates act centrally, decreasing vascular tone and slowing the heart rate, and acts peripherally to block alpha-receptors. One other possible mechanism is the effect of ergoloid mesylates on neuronal cell metabolism, resulting in improved oxygen uptake and cerebral metabolism, thereby normalizing depressed neurotransmitter levels.
75	<chem>CN1CCC23c4c5ccc(c4OC2C(CCC3C1C5)O)OC</chem>	DIHYDROCODEINE	It is prescribed for pain, severe dyspnea, or as an antitussive, either alone or compounded with aspirin or paracetamol, as in co-dydramol. Developed in Germany.	It is a cough suppressant that affects the signals in the brain that trigger cough reflex.
76	<chem>CN(C)CCOC(c1ccccc1)c2ccccc2</chem>	DIPHENHYDRAMINE	For the treatment of symptoms associated with Vertigo/Meniere's disease, nausea and vomiting, motion sickness and insect bite.	This anticholinergic action appears to be due to a central antimuscarinic effect, which also may be responsible for its antiemetic effects, although the exact mechanism is unknown.

77	<chem>CCC(=O)C(CC(C)N1CCCC1)(c2ccccc2)c3ccccc3</chem>	DIPIPANONE	Used for very severe pain in cases where morphine is indicated but cannot be used due to the patient being allergic to morphine. It is approved in UK.	Dipipanone is an extremely strong opioid
78	<chem>COc1cc2c(cc1OC)C(=O)C(C2)CC3CCN(CC3)Cc4ccccc4</chem>	DONEPEZIL	For the palliative treatment of mild to moderate dementia of the Alzheimer's type	Donepezil is a piperidine derivative that is a centrally active, reversible inhibitor of acetylcholinesterase.
79	<chem>CN(C)CC/C=C/1\c2ccc(cc2)Cc3ccccc3</chem>	DOSULEPIN	Dosulepin is relatively mild and is used for low-level anxiety, depression and similar disorders, as well as the treatment of chronic and ongoing pain disorders, particularly where insomnia and/or loss of appetite are present.	Dosulepin blocks the reuptake of serotonin and norepinephrine in the brain, thereby increasing their levels. It is believed that this action is responsible for its mood-elevating effects.
80	<chem>CCN1CC(C(C1=O)(c2ccccc2)c3ccccc3)CCN4CCOCC4</chem>	DOXAPRAM	Doxapram is used in intensive care settings to stimulate the respiratory rate in patients with respiratory failure. It may be useful for treating respiratory depression in patients who have taken excessive doses of drugs such as buprenorphine which may fail to respond adequately to treatment with naloxone	Doxapram stimulates chemoreceptors in the carotid arteries, which in turn, stimulates the respiratory centre in the brain stem.

81	<chem>CN(C)CC/C=C\1/c2ccc cc2COc3c1cccc3</chem>	DOXEPIN	Approved uses may vary by country. In the United States, the FDA approved the use of doxepin in the treatment of depression as well as insomnia.	Doxepin inhibits the reuptake of serotonin and norepinephrine. Its actions of the reuptake of dopamine are negligible.
82	<chem>CC(c1ccccc1)(c2cccn 2)OCCN(C)C</chem>	DOXYLAMINE	Used alone as a short-term sleep aid, in combination with other drugs as a night-time cold and allergy relief drug.	Like other antihistamines, doxylamine acts by competitively inhibiting histamine at H1 receptors. It also has substantial sedative and anticholinergic effects.
83	<chem>c1ccc2c(c1)[nH]c(=O)n 2C3=CCN(CC3)CCCC(=O)c4ccc(cc4)F</chem>	DROPERIDOL	Droperidol is used to produce tranquilization and to reduce the incidence of nausea and vomiting in surgical and diagnostic procedures.	The exact mechanism of action is unknown, however, droperidol causes a CNS depression at subcortical levels of the brain, midbrain, and brainstem reticular formation.
84	<chem>c1cc(c(cc1C(C(C(=O)O)N)O)O)O</chem>	DROXIDOPA	For treatment of neurogenic orthostatic hypotension (NOH) associated with various disorders including Multiple System Atrophy, Familial Amyloid Polyneuropathy, hemodialysis induced hypotension and Parkinson's Disease.	Droxidopa crosses the blood-brain barrier where it is converted to norepinephrine via decarboxylation by L-aromatic-amino-acid decarboxylase. Increased levels of norepinephrine in the central nervous system (CNS) may be beneficial to patients in a wide range of indications.
85	<chem>CC(C(c1ccccc1)O)NC</chem>	EPHEDRINE	Ephedrine commonly used as a stimulant, appetite suppressant, concentration aid, decongestant, and to treat hypotension associated with anaesthesia.	Ephedrine is a sympathomimetic amine - that is, its principal mechanism of action relies on its direct and indirect actions on the adrenergic receptor system, which is part of the sympathetic nervous system.

86	<chem>c1ccc(cc1)C2=NCc3nncn3-c4c2cc(cc4)Cl</chem>	ESTAZOLAM	For the short-term management of insomnia characterized by difficulty in falling asleep, frequent nocturnal awakenings, and/or early morning awakenings.	Benzodiazepines bind nonspecifically to benzodiazepine receptors, which affects muscle relaxation, anticonvulsant activity, motor coordination, and memory.
87	<chem>CCN(CC)C(C)CN1c2ccccc2Sc3c1cccc3</chem>	ETHOPROPAZINE	For use in the treatment of Parkinson's disease and also used to control severe reactions to certain medicines such as reserpine.	Ethopropazine's antiparkinson action can be attributed to its anticholinergic properties. Ethopropazine partially blocks central (striatal) cholinergic receptors, thereby helping to balance cholinergic and dopaminergic activity in the basal ganglia.
88	<chem>CCC1(CC(=O)NC1=O)C</chem>	ETHOSUXIMIDE	For the treatment of petit mal epilepsy.	Binds to T-type voltage sensitive calcium channels. T-type channels serve pacemaking functions in both central neurons and cardiac nodal cells and support calcium signaling in secretory cells and vascular smooth muscle.
89	<chem>CCN1C(=O)C(NC1=O)c2ccccc2</chem>	ETHOTOIN	An anticonvulsant drug used in the treatment of epilepsy.	Ethotoin exerts an antiepileptic effect without causing general central nervous system depression. The mechanism of action is probably to stabilize rather than to raise the normal seizure threshold, and to prevent the spread of seizure activity rather than to abolish the primary focus of seizure discharges
90	<chem>c1ccc(cc1)C(COC(=O)N)COC(=O)N</chem>	FELBAMATE	An anticonvulsant drug used in the treatment of epilepsy.	As with many anticonvulsants, the precise mechanism is unknown. It has an effect on GABA receptor binding sites. It may also work as a NMDA receptor antagonist.

91	<chem>CCC(=O)N(c1ccccc1)C2CCN(CC2)CCc3ccccc3</chem>	FENTANYL	For the treatment of cancer patients with severe pain that breaks through their regular narcotic therapy.	Fentanyl interacts predominately with the opioid mu-receptor but also binds to kappa and delta-type opioid receptors. These mu-binding sites are discretely distributed in the human brain, spinal cord, and other tissues. In clinical settings, Fentanyl exerts its principal pharmacologic effects on the central nervous system.
92	<chem>CCOC(=O)c1c2n(cn1)-c3ccc(cc3C(=O)N(C2)C)F</chem>	FLUMAZENIL	For the complete or partial reversal of the sedative effects of benzodiazepines in cases where general anesthesia has been induced and/or maintained with benzodiazepines, and where sedation has been produced with benzodiazepines for diagnostic and therapeutic procedures.	Flumazenil, an imidazobenzodiazepine derivative, antagonizes the actions of benzodiazepines on the central nervous system. Flumazenil competitively inhibits the activity at the benzodiazepine recognition site on the GABA/benzodiazepine receptor complex.
93	<chem>c1ccc(cc1)/C=C/CN2C(CN(CC2)C(c3ccc(cc3)F)c4ccc(cc4)F</chem>	FLUNARIZINE	Used in the prophylaxis of migraine, occlusive peripheral vascular disease, vertigo of central and peripheral origin, and as an adjuvant in the therapy of epilepsy.	Flunarizine has H1-receptor blocking action and calcium-channel blocking effect. It is said to be the only calcium antagonist able to protect brain cells against hypoxic damage. In addition, the considerable body of information which shows flunarizine capable of directly influencing the central nervous system, suggests that the drug's anti-migraine action may depend on its ability to influence central phenomena.

94	<chem>CN1c2ccc(cc2C(=NCC1=O)c3ccccc3F)[N+](=O)[O-]</chem>	FLUNITRAZEPAM	For short-term treatment of severe insomnias, that are not responsive to other hypno	Benzodiazepines bind nonspecifically to benzodiazepine receptors BNZ1, which mediates sleep, and BNZ2, which affects muscle relaxation, anticonvulsant activity, motor coordination, and memory.
95	<chem>CNCCC(c1ccccc1)Oc2ccc(cc2)C(F)(F)F</chem>	FLUOXETINE	For the treatment of depression, obsessive compulsive disorder, and bulimia nervosa.	Metabolized to norfluoxetine, fluoxetine is a selective serotonin-reuptake inhibitor (SSRI), it blocks the reuptake of serotonin at the serotonin reuptake pump of the neuronal membrane, enhancing the actions of serotonin on 5HT1A autoreceptors.
96	<chem>c1ccc2c(c1)/C(=C\CCN3CCN(CC3)CCO)/c4cc(ccc4S2)C(F)(F)F</chem>	FLUPENTHIXOL	For use in the treatment of schizophrenia and depression	The mechanism of action of Flupenthixol is not completely understood. Flupenthixol is a powerful antagonist of both D1 and D2 dopamine receptors, and an alpha-adrenergic receptor antagonist. It's antipsychotic activity is thought to be related to blocks postsynaptic dopamine receptors in the CNS.
97	<chem>c1ccc2c(c1)N(c3cc(ccc3S2)C(F)(F)F)CCCN4CCN(CC4)CCO</chem>	FLUPHENAZINE	For management of manifestations of psychotic disorders.	Fluphenazine blocks postsynaptic mesolimbic dopaminergic D1 and D2 receptors in the brain; depresses the release of hypothalamic and hypophyseal hormones and is believed to depress the reticular activating system thus affecting basal metabolism, body temperature, wakefulness, vasomotor tone, and emesis.
98	<chem>CCOC(=O)Nc1ccc(nc1N)NCc2ccc(cc2)F</chem>	FLUPIRTINE	It is used as an analgesic for acute and chronic pain, mainly for moderate to severe pain.	It is a centrally acting nonopioid analgesic. It is available in Europe since 1984 and sold mainly under the names Katadolon, Trancolong and Metanor. It is unique as a non-opioid, non-NSAID, non-steroidal analgesic.

99	<chem>CCN(CC)CCN1c2ccc(c2C(=NCC1=O)c3cccc3F)Cl</chem>	FLURAZEPAM	For short-term and intermittent use in patients with recurring insomnia and poor sleeping habits	The main pharmacological effect of flurazepam is to increase the effect of GABA at the GABA-A receptor via binding to the benzodiazepine site on the GABA-A receptor causing an increase influx of chloride ions into the GABA-A neuron. Flurazepam is a unique benzodiazepine in that it is a partial agonist of benzodiazepine receptors whereas other benzodiazepines are full agonists of benzodiazepine receptors.
100	<chem>c1ccc(cc1)N2CNC(=O)C23CCN(CC3)CCCC(c4ccc(cc4)F)c5ccc(cc5)F</chem>	FLUSPIRILENE	Used for the treatment of schizophrenia.	A dopamine D2 receptor antagonist which is a long-acting neuroleptic useful in the maintenance therapy of schizophrenic patients, also displays Ca ²⁺ channel blocking activity. In clinical trials, the low incidence of seizures provoked by fluspirilene might be related to its intrinsic ability to inhibit synaptic transmission and epileptiform activity.
101	<chem>c1ccc(c(c1)C2=NCC(=O)N(c3c2cc(cc3)Cl)CC4CC4)F</chem>	FLUTOPRAZEPAM	Flutoprazepam is typically used for the treatment of severe insomnia and may also be used for treating stomach ulcers.	Flutoprazepam is a benzodiazepine derivative. It was discovered in Japan in 1972, and its mostly confined to that country even today. Flutoprazepam is around four times more potent by weight compared to diazepam.
102	<chem>COCCCC/C(=N\OCCN)/c1ccc(cc1)C(F)(F)F</chem>	FLUVOXAMINE	For management of depression and for Obsessive Compulsive Disorder (OCD). Has also been used in the management of bulimia nervosa.	The exact mechanism of action of fluvoxamine has not been fully determined, but appears to be linked to its inhibition of CNS neuronal uptake of serotonin. Fluvoxamine blocks the reuptake of serotonin at the serotonin reuptake pump of the neuronal membrane, enhancing the actions of serotonin on 5HT _{1A} autoreceptors.

103	<chem>C1CCC(CC1)(CC(=O)O)CN</chem>	GABAPENTIN	For the management of postherpetic neuralgia in adults and as adjunctive therapy in the treatment of partial seizures with and without secondary generalization in patients over 12 years of age with epilepsy.	Gabapentin interacts with cortical neurons at auxiliary subunits of voltage-sensitive calcium channels. Gabapentin increases the synaptic concentration of GABA, enhances GABA responses at non-synaptic sites in neuronal tissues, and reduces the release of mono-amine neurotransmitters.
104	<chem>CN1CCC23C=CC(CC2Oc4c3c(ccc4OC)C1)O</chem>	GALANTAMINE	For the treatment of mild to moderate dementia of the Alzheimer's type.	Galantamine's proposed mechanism of action involves the reversible inhibition of acetylcholinesterase, which prevents the hydrolysis of acetylcholine, leading to an increased concentration of acetylcholine at cholinergic synapses.
105	<chem>Cn1c2ccccc2c(n1)C(=O)NC3CC4CCCC(C3)N4C</chem>	GRANISETRON	For the prevention of nausea and vomiting associated with initial and repeat courses of emetogenic cancer therapy (including high dose cisplatin), postoperation, and radiation (including total body irradiation and daily fractionated abdominal radiation).	Granisetron is a potent, selective antagonist of 5-HT ₃ receptors. The antiemetic activity of the drug is brought about through the inhibition of 5-HT ₃ receptors present both centrally (medullary chemoreceptor zone) and peripherally (GI tract).
106	<chem>c1ccc(cc1)C2=NCC(=O)N(c3c2cc(cc3)Cl)CC(F)(F)F</chem>	HALAZEPAM	Used to relieve anxiety, nervousness, and tension associated with anxiety disorders.	Central nervous system agents of the 1,4-benzodiazepine class presumably exert their effects by binding at stereo specific receptors at several sites within the central nervous system. Their exact mechanism of action is unknown. Clinically, all benzodiazepines cause a dose-related central nervous system depressant activity varying from mild impairment of task performance to hypnosis.

107	<chem>c1cc(ccc1C(=O)CCCN2CCC(CC2)(c3ccc(cc3)Cl)O)F</chem>	HALOPERIDOL	For the management of psychotic disorders (eg. schizophrenia) and delirium, as well as to control tics and vocal utterances of Tourette's syndrome (Gilles de la Tourette's syndrome). Also used for the treatment of severe behavioural problems in children with disruptive behaviour disorder or ADHD.	The precise mechanism whereby the therapeutic effects of haloperidol are produced is not known, but the drug appears to depress the CNS at the subcortical level of the brain, midbrain, and brain stem reticular formation.
108	<chem>CN1CCC23c4c5ccc(c4OC2C(=O)CCC3C1C5)OC</chem>	HYDROCODONE	For relief of moderate to moderately severe pain. Also used for the symptomatic relief of nonproductive cough, alone or in combination with other antitussives or expectorants.	Hydrocodone acts as a weak agonist at OP1, OP2, and OP3 opiate receptors within the central nervous system (CNS). Hydrocodone primarily affects OP3 receptors, which are coupled with G-protein receptors and function as modulators, both positive and negative, of synaptic transmission via G-proteins that activate effector proteins
109	<chem>CN1CCC23c4c5ccc(c4OC2C(=O)CCC3C1C5)O</chem>	HYDROMORPHONE	For the relief of moderate to severe pain such as that due to surgery, cancer, trauma/injury, or burns.	Hydromorphone is a narcotic analgesic; its principal therapeutic effect is relief of pain. Hydromorphone interacts predominantly with the opioid mu-receptors. These mu-binding sites are discretely distributed in the human brain, with high densities in the posterior amygdala, hypothalamus, thalamus, nucleus caudatus, putamen, and certain cortical areas.

110	<chem>c1ccc(cc1)C(c2ccc(cc2)Cl)N3CCN(CC3)CCOCCO</chem>	HYDROXYZINE	For symptomatic relief of anxiety and tension associated with psychoneurosis and as an adjunct in organic disease states in which anxiety is manifested. Useful in the management of pruritus due to allergic conditions such as chronic urticaria.	Hydroxyzine competes with histamine for binding at H1-receptor sites on the effector cell surface, resulting in suppression of histaminic edema, flare, and pruritus. The sedative properties of hydroxyzine occur at the subcortical level of the CNS. Secondary to its central anticholinergic actions, hydroxyzine may be effective as an antiemetic.
111	<chem>CN1C2CC(CC1C3C2O3)OC(=O)C(CO)c4cccc4</chem>	SCOPOLAMINE	For the treatment of excessive salivation, colicky abdominal pain, bradycardia, sialorrhoea, diverticulitis, irritable bowel syndrome and motion sickness.	Scopolamine acts by interfering with the transmission of nerve impulses by acetylcholine in the parasympathetic nervous system (specifically the vomiting center).
112	<chem>CC1=C(C(=O)C(=C(C1=O)OC)OC)CCCCCCC</chem>	IDEBENONE	Nootropic effects and Alzheimer's disease	It is a brain stimulant that increases brain energy levels and rejuvenates cell mitochondria throughout the whole body. Most recently, it has been shown to be very supportive in the treatment of Friedreich's ataxia and Duchenne muscular dystrophy.
113	<chem>CC(C(c1ccc(cc1)O)O)N2CCC(CC2)Cc3ccccc3</chem>	IFENPRODIL	is a clinically used cerebral vasodilator approved in Japan	It interacts with several receptors, such as 1 adrenergic, N-methyl-D-aspartate, serotonin and receptors.

114	<chem>CN(C)CCCN1c2ccccc2CCc3c1cccc3</chem>	IMIPRAMINE	is an antidepressant medication, a tricyclic antidepressant of the dibenzazepine group. Imipramine is mainly used in the treatment of major depression and enuresis (inability to control urination).	Imipramine works by inhibiting the neuronal re-uptake of the neurotransmitters norepinephrine and serotonin. It binds the sodium-dependent serotonin transporter and sodium-dependent norepinephrine transporter preventing or reducing the reuptake of norepinephrine and serotonin by nerve cells.
115	<chem>c1cc2c(c(c1)OCC3CNCCO3)CC=C2</chem>	INDELOXAZINE	cerebral activator used in Japan for the treatment of cerebrovascular disease	Indeloxazine acts as a serotonin releasing agent and norepinephrine reuptake inhibitor.[3] It also acts as an NMDA receptor antagonist. It enhances acetylcholine release through indirect activation of the 5-HT ₄ receptor. Indeloxazine has nootropic, neuroprotective, anticonvulsant, and antidepressant effects.
116	<chem>Cc1cc(no1)C(=O)NNC2CCCCC2</chem>	ISOCARBOXAZID	May be used to treat major depressive disorder.	Isocarboxazid works by irreversibly blocking the action of a chemical substance known as monoamine oxidase (MAO) in the nervous system. MAO subtypes A and B are involved in the metabolism of serotonin and catecholamine neurotransmitters such as epinephrine, norepinephrine, and dopamine. Isocarboxazid, as a nonselective MAO inhibitor, binds irreversibly to monoamine oxidase-A (MAO-A) and monoamine oxidase-B (MAO-B). The reduced MAO activity results in an increased concentration of these neurotransmitters in storage sites throughout the central nervous system (CNS) and sympathetic nervous system. This increased availability of one or more

				monoamines is the basis for the antidepressant activity of MAO inhibitors.
117	<chem>CC1=CC(=O)N2CC(=O)N(c3ccc(cc3C2(O1)c4ccccc4)Cl)C</chem>	KETAZOLAM	Ketazolam could be used for the treatment of anxiety. In approved countries, it is indicated for the treatment of anxiety, tension, irritability and similar stress related symptoms.	Benzodiazepines share a similar chemical structure and their effects in humans are mainly produced by the allosteric modification of a specific kind of neurotransmitter receptor, the GABAA receptor, which increases the conductance of this inhibitory channel; this results in the various therapeutic effects.
118	<chem>c1cc(c(c(c1)Cl)Cl)c2c(nc(n2)N)N</chem>	LAMOTRIGINE	For the adjunctive treatment of partial seizures in epilepsy and generalized seizures of Lennox-Gastaut syndrome. Also for the maintenance treatment of bipolar I disorder and depression.	One proposed mechanism of action of Lamotrigine, the relevance of which remains to be established in humans, involves an effect on sodium channels. in vitro pharmacological studies suggest that lamotrigine inhibits voltage-sensitive sodium channels and/or calcium channels, thereby stabilizing neuronal membranes and consequently modulating presynaptic transmitter release of excitatory amino acids (e.g., glutamate and aspartate).

119	<chem>C=CCN1CCC23CCCCC2C1Cc4c3cc(cc4)O</chem>	LEVALLORPHAN	For the complete or partial reversal of narcotic depression, including respiratory depression, induced by opioids.	Levallorphan antagonizes opioid effects by competing for the same receptor sites. It binds to the opioid mu receptor and the nicotinic acetylcholine receptor alpha2/alpha3.
120	<chem>CCC(C(=O)N)N1CCCC1=O</chem>	LEVETIRACETAM	Used as adjunctive therapy in the treatment of partial onset seizures in adults and children 4 years of age and older with epilepsy.	The exact mechanism by which levetiracetam acts to treat epilepsy is unknown. However, the drug binds to a synaptic vesicle protein, SV2A, which is believed to impede nerve conduction across synapses.
121	<chem>c1cc(c(cc1CC(C(=O)O)N)O)O</chem>	LEVODOPA	For the treatment of idiopathic Parkinson's disease (Paralysis Agitans), postencephalitic parkinsonism, symptomatic parkinsonism	Striatal dopamine levels in symptomatic Parkinson's disease are decreased by 60 to 80%, striatal dopaminergic neurotransmission may be enhanced by exogenous supplementation of dopamine through administration of dopamine's precursor, levodopa. A small percentage of each levodopa dose crosses the blood-brain barrier and is decarboxylated to dopamine.
122	<chem>CC(CN1c2ccccc2Sc3c1cc(cc3)OC)CN(C)C</chem>	METHOTRIMEPRAZINE	For the treatment of psychosis, particular those of schizophrenia, and manic phases of bipolar disorder.	Methotrimeprazine's antipsychotic effect is largely due to its antagonism of dopamine receptors in the brain. In addition, its binding to 5HT2 receptors may also play a role.
123	<chem>CN1CCC23CCCCC2C1Cc4c3cc(cc4)O</chem>	LEVORPHANOL	For the management of moderate to severe pain or as a preoperative medication where an opioid analgesic is appropriate.	Like other mu-agonist opioids it is believed to act at receptors in the periventricular and periaqueductal gray matter in both the brain and spinal cord to alter the transmission and perception of pain.

124	<chem>CN(CCCN1c2ccccc2Cc3c1cccc3)CC(=O)c4ccc(cc4)Cl</chem>	LOFEPRAMINE	In the United Kingdom, lofepramine is licensed for the treatment of depression.	It was hypothesized that the action of this combined therapy may relate to activation of the noradrenergic locus coeruleus/lateral tegmentum (LC/LT) system which has the potential to influence the functioning of large areas of the brain and spinal cord.
125	<chem>CC(C1=NCCN1)Oc2c(cccc2Cl)Cl</chem>	LOFEXIDINE	Treatment in addictions and substance abuse.	Lofexidine is an alpha2-adrenergic receptor agonist.
126	<chem>CN1CCN(CC1)/C=C\2/C(=O)N3c4ccc(cc4C(=NCC3=N2)c5ccccc5Cl)[N+](=O)[O-]</chem>	LOPRAZOLAM	It is licensed and marketed for the short term treatment of moderately severe insomnia.	Loprazolam is a benzodiazepine, which acts via positively modulating the GABAA receptor complex via a binding to the benzodiazepine receptor which is situated on alpha subunit containing GABAA receptors.
127	<chem>c1ccc(c(c1)C2=NC(C(=O)Nc3c2cc(cc3)Cl)O)Cl</chem>	LORAZEPAM	For the management of anxiety disorders, and for treatment of status epilepticus.	Lorazepam binds to an allosteric site on GABA-A receptors, which are pentameric ionotropic receptors in the CNS.
128	<chem>CN1c2ccc(cc2C(=NC(C1=O)O)c3ccccc3Cl)Cl</chem>	LORMETAZEPAM	Lormetazepam is considered a hypnotic benzodiazepine and is officially indicated for moderate to severe insomnia. It was not approved in United States.	Lormetazepam and other benzodiazepine drugs act as positive modulators at the GABAA benzodiazepine receptor complex.

129	<chem>CN1CCN(CC1)C2=Nc3cccc3Oc4c2cc(cc4)Cl</chem>	LOXAPINE	For the management of the manifestations of psychotic disorders such as schizophrenia.	Loxapine is a dopamine antagonist, and also a serotonin 5-HT ₂ blocker.
130	<chem>CCN(CC)C(=O)NC1CN(C2Cc3c[nH]c4c3c(ccc4)C2=C1)C</chem>	LYSURIDE	For the management of Parkinson's Disease	Lisuride is an anti-Parkinson drug chemically related to the dopaminergic ergoline Parkinson's drugs. Lisuride binds to the 5-HT(1A) and 5-HT(2A/2C) receptors. It is also thought to bind to the dopamine receptor and to act as a dopamine agonist.
131	<chem>CNCCCC12CCC(c3c1cccc3)c4c2cccc4</chem>	MAPROTILINE	For treatment of depression, including the depressed phase of bipolar depression, psychotic depression, and involutional melancholia, and may also be helpful in treating certain patients suffering severe depressive neurosis.	Maprotiline exerts its antidepressant action by inhibition of presynaptic uptake of catecholamines, thereby increasing their concentration at the synaptic clefts of the brain.
132	<chem>c1ccc2c(c1)C3=NCCN3C2(c4ccc(cc4)Cl)O</chem>	MAZINDOL	Mazindol is used in short-term (i.e., a few weeks) treatment of exogenous obesity.	Mazindol is a sympathomimetic amine, which is similar to amphetamine. It stimulates the central nervous system, which increases heart rate and blood pressure, and decreases appetite.
133	<chem>Cc1cccc(c1)CN2CCN(CC2)C(c3cccc3)c4ccc(cc4)Cl</chem>	MECLIZINE/MECLOZINE	For the prevention and treatment of nausea, vomiting, or dizziness associated with motion sickness.	Along with its actions as an antagonist at H ₁ -receptors, meclizine also possesses anticholinergic, central nervous system depressant, and local anesthetic effects.

134	<chem>CC12CC3CC(C1)(CC(C3)(C2)N)C</chem>	MEMANTINE	For the treatment of moderate to severe dementia of the Alzheimer's type.	Memantine is a low-affinity voltage-dependent uncompetitive antagonist at glutamatergic NMDA receptors.[14][15] By binding to the NMDA receptor with a higher affinity than Mg ²⁺ ions, memantine is able to inhibit the prolonged influx of Ca ²⁺ ions, which forms the basis of neuronal excitotoxicity.
135	<chem>CCC1(C(=O)N(C(=O)N1)C)c2ccccc2</chem>	MEPHENYTOIN	For the treatment of refractory partial epilepsy.	Its main mechanism is to block frequency-, use- and voltage-dependent neuronal sodium channels, and therefore limit repetitive firing of action potentials. The primary site of action appears to be the motor cortex where spread of seizure activity is inhibited.
136	<chem>CCCC(C)(COC(=O)N)COC(=O)N</chem>	MEPROBAMATE	For the management of anxiety disorders or for the short-term relief of the symptoms of anxiety.	It has been shown in animal studies to have effects at multiple sites in the central nervous system, including the thalamus and limbic system. Meprobamate binds to GABAA receptors which interrupt neuronal communication in the reticular formation and spinal cord, causing sedation and altered perception of pain
137	<chem>CCC1(CCCCN(C1)C)c2cccc(c2)O</chem>	MEPTAZINOL	Meptazinol (trade name Meptid) is an opioid analgesic for use with moderate to severe pain, most commonly used to treat pain in obstetrics (childbirth).	A partial μ -opioid receptor agonist, its mixed agonist/antagonist activity affords it a lower risk of dependence and abuse than full μ agonists like morphine.
138	<chem>CN(C)CCN(Cc1ccc(cc1)OC)c2ccccc2</chem>	MEPYRAMINE	Mepyramine is a first generation antihistamine used in treating allergies, symptomatic relief of hypersensitivity reaction, and in pruritic skin disorders.	It rapidly permeates the brain often causing drowsiness. It also has anticholinergic properties.

139	<chem>CN1CCCC1CCN2c3cccc3Sc4c2cc(cc4)S(=O)C</chem>	MESORIDAZINE	Used in the treatment of schizophrenia, organic brain disorders, alcoholism and psychoneuroses.	Mesoridazine, as with other phenothiazines, acts indirectly on reticular formation, whereby neuronal activity into reticular formation is reduced without affecting its intrinsic ability to activate the cerebral cortex.
140	<chem>CC1(CC(=O)N(C1=O)C)c2ccccc2</chem>	MESUXIMIDE	For the control of absence (petit mal) seizures that are refractory to other drugs.	Binds to T-type voltage sensitive calcium channels. T-type channels serve pacemaking functions in both central neurons and cardiac nodal cells and support calcium signaling in secretory cells and vascular smooth muscle.
141	<chem>CN1c2ccc(cc2C(=NCC1COC)c3ccccc3Cl)Br</chem>	METACLAZEPAM	It is a relatively selective anxiolytic with less sedative or muscle relaxant properties than other benzodiazepines such as diazepam or bromazepam	It is a benzodiazepine derivative, marketed under the brand name Talis. It is manufactured by Organon, Ger. Benzodiazepines have been shown to bind and modulate the major GABA receptor in the brain.
142	<chem>Cc1cc(cc(c1)OCC2CN C(=O)O2)C</chem>	METAXALONE	It is a muscle relaxant used to relax muscles and relieve pain caused by strains, sprains, and other musculoskeletal conditions.	The mechanism of action of metaxalone in humans has not been established, but may be due to general central nervous system depression.
143	<chem>CCC(=O)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2</chem>	METHADONE	For the treatment of dry cough, drug withdrawal syndrome, opioid type drug dependence, and pain.	Methadone is a mu-agonist; a synthetic opioid analgesic with multiple actions qualitatively similar to those of morphine, the most prominent of which involves the central nervous system and organs composed of smooth muscle.

144	<chem>CC(Cc1ccccc1)NC</chem>	METHAMPHETAMINE	For the treatment of Attention Deficit Disorder with Hyperactivity (ADHD) and exogenous obesity.	Methamphetamine enters the brain and triggers a cascading release of norepinephrine, dopamine and serotonin.
145	<chem>CN1CCC(C1)CN2c3ccccc3Sc4c2ccccc4</chem>	METHDILAZINE	Used for the symptomatic relief of hypersensitivity reactions and particularly for the control of pruritic skin disorders.	Methdilazine (Dilosyn, Tacaryl) is a first-generation antihistamine with anticholinergic properties of the phenothiazine class.
146	<chem>COc1ccccc1OCC(COC(=O)N)O</chem>	METHOCARBAMOL	For use as an adjunct to rest, physical therapy, and other measures for the relief of discomforts associated with acute, painful musculoskeletal conditions.	The mechanism of action of methocarbamol in humans has not been established, but may be due to central nervous system depression. It has no direct action on the contractile mechanism of striated muscle, the motor end plate or the nerve fiber.
147	<chem>CCC1(C(=O)NC(=O)N(C1=O)C)c2ccccc2</chem>	METHYLPHENOBARBITAL	For the relief of anxiety, tension, and apprehension, also used as an anticonvulsant for the treatment of epilepsy.	Methylphenobarbital binds at a distinct binding site associated with a Cl ⁻ ionopore at the GABAA receptor, increasing the duration of time for which the Cl ⁻ ionopore is open. The post-synaptic inhibitory effect of GABA in the thalamus is, therefore, prolonged.
148	<chem>CC1CC2C3CCC(C3(C(C2C4(C1=CC(=O)C=C4)C)O)C)(C(=O)CO)O</chem>	METHYLPREDNISOLONE	Like most adrenocortical steroids, methylprednisolone is typically used for its anti-inflammatory effects.	The antiinflammatory actions of corticosteroids are thought to involve phospholipase A2 inhibitory proteins, lipocortins, which control the biosynthesis of potent mediators of inflammation such as prostaglandins and leukotrienes. has some serious side effects if taken long-term, including weight gain, glaucoma, osteoporosis and psychosis. It is also on trial for primary CNS non-Hodgkin

				lymphoma.
149	<chem>CCC(CO)NC(=O)C1CN(C2Cc3cn(c4c3c(ccc4)C2=C1)C)C</chem>	METHYSERGIDE	For the treatment of vascular headache	Methysergide is serotonin antagonists acts on central nervous system (CNS), which directly stimulates the smooth muscle leading to vasoconstriction.
150	<chem>CCN(CC)CCNC(=O)c1cc(c(cc1OC)N)Cl</chem>	METOCLOPRAMIDE	For the treatment of gastroesophageal reflux disease (GERD). It is also used in treating nausea and vomiting, and to increase gastric emptying.	It appears to bind to dopamine D2 receptors where it is a receptor antagonist, and is also a mixed 5-HT3 receptor antagonist/5-HT4 receptor agonist. The anti-emetic action of metoclopramide is due to its antagonist activity at D2 receptors in the chemoreceptor trigger zone (CTZ) in the CNS.
151	<chem>CN1CCN2c3ccccc3Cc4ccccc4C2C1</chem>	MIANSERIN	For the treatment of depression.	Mianserin is an antagonist at the H1, 5-HT1D, 5-HT2A, 5-HT2C, 5-HT3, 5-HT6, 5-HT7, α 1-adrenergic, and α 2-adrenergic receptors, and also acts as a norepinephrine reuptake inhibitor (NRI) via blockade of the norepinephrine transporter (NET).
152	<chem>Cc1ncc2n1-c3ccc(cc3C(=NC2)c4ccccc4F)Cl</chem>	MIDAZOLAM	For use as a sedative perioperatively.	It is thought that the actions of benzodiazepines such as midazolam are mediated through the inhibitory neurotransmitter gamma-aminobutyric acid (GABA), which is one of the major inhibitory neurotransmitters in the brain.

153	<chem>CCN(CC)C(=O)C1(CC1CN)c2ccccc2</chem>	MILNACIPRAN	Milnacipran is used to treat moderate to severe clinical depression and chronic pain.	Milnacipran inhibits norepinephrine and serotonin reuptake in a 3:1 ratio, in practical use this means a balanced (equal) action upon both transmitters.
154	<chem>CN1CCN2c3c(cccn3)Cc4ccccc4C2C1</chem>	MIRTAZAPINE	For the treatment of major depressive disorder.	Mirtazapine acts as an antagonist at central pre-synaptic alpha(2)-receptors, inhibiting negative feedback to the presynaptic nerve and causing an increase in NE release.
155	<chem>c1cc(ccc1C(=O)NCCN2CCOCC2)Cl</chem>	MOCLOBEMIDE	For the treatment of depression.	The mechanism of action of moclobemide involves the selective, reversible inhibition of MAO-A. This inhibition leads to a decrease in the metabolism and destruction of monoamines in the neurotransmitters.
156	<chem>c1ccc(cc1)C(c2ccccc2)S(=O)(=O)CC(=O)N</chem>	MODAFINIL	To improve wakefulness in patients with excessive daytime sleepiness (EDS) associated with narcolepsy.	The exact mechanism of action is unclear, although in vitro studies have shown it to inhibit the reuptake of dopamine by binding to the dopamine reuptake pump, and lead to an increase in extracellular dopamine.
157	<chem>CCc1c([nH])c2c1C(=O)C(CC2)CN3CCOCC3</chem>	MOLINDONE	Molindone is used for the management of the manifestations of psychotic disorders.	The exact mechanism has not been established, however, based on electroencephalogram (EEG) studies, molindone is thought to act by occupying (antagonizing) dopamine (D2) receptor sites in the reticular limbic systems in the brain, thus decreasing dopamine activity.

158	<chem>CN1CCC23c4c5ccc(c4OC2C(C=CC3C1C5)O)O</chem>	MORPHINE	For the relief and treatment of severe pain.	The precise mechanism of the analgesic action of morphine is unknown. However, specific CNS opiate receptors have been identified and likely play a role in the expression of analgesic effects. Morphine first acts on the mu-opioid receptors.
159	<chem>CCCCCCC(C)(C)c1cc(c2c(c1)OC(C3C2CC(=O)CC3)(C)C)O</chem>	NABILONE	Used for the control of nausea and vomiting, caused by chemotherapeutic agents used in the treatment of cancer, in patients who have failed to respond adequately to conventional antiemetic treatments.	Nabilone (agonist) activates CB1 receptors—which reduces proemetic signaling in the vomit center and thus inhibits nausea and vomiting.
160	<chem>c1cc(c2c3c1CC4C5(C3(CCN4CC6CCC6)C(O2)C(CC5)O)O)O</chem>	NALBUPHINE	For the relief of moderate to severe pain.	is believed to interact with an opiate receptor site in the CNS (probably in or associated with the limbic system).
161	<chem>C=C1CCC2(C3Cc4ccc(c5c4C2(C1O5)CCN3CC6CC6)O)O</chem>	NALMEFENE	Nalmefene (Revex) is an opioid receptor antagonist used primarily in the management of alcohol dependence, and also has been investigated for the treatment of other addictions such as pathological gambling and addiction to shopping.	an opioid receptor antagonist

162	<chem>C=CCN1CCC23c4c5cc c(c4OC2C(=O)CCC3(C 1C5)O)O</chem>	NALOXONE	For the complete or partial reversal of narcotic depression, including respiratory depression, induced by opioids including natural and synthetic narcotics, propoxyphene, methadone and the narcotic-antagonist analgesics: nalbuphine, pentazocine and butorphanol.	preponderance of evidence suggests that naloxone antagonizes the opioid effects by competing for the same receptor sites, especially the opioid mu receptor. Recently, naloxone has been shown to bind all three opioid receptors (mu, kappa and gamma) but the strongest binding is to the mu receptor.
163	<chem>c1cc(c2c3c1CC4C5(C3 (CCN4CC6CC6)C(O2) C(=O)CC5)O)O</chem>	NALTREXONE	an adjunct to a medically supervised behaviour modification program in the maintenance of opiate cessation	Naltrexone is a pure opiate antagonist and has little or no agonist activity. Naltrexone is thought to act as a competitive antagonist at mc, κ, and δ receptors in the CNS, with the highest affinity for the μ receptor.
164	<chem>CCc1nn(c(=O)n1CCOc 2ccccc2)CCCN3CCN(CC3)c4cccc(c4)Cl</chem>	NEFAZODONE	For the treatment of depression	Within the serotonergic system, nefazodone acts as an antagonist at type 2 serotonin (5-HT ₂) post-synaptic receptors and, like fluoxetine-type antidepressants, inhibits pre-synaptic serotonin (5-HT) reuptake. These mechanisms increase the amount of serotonin available to interact with 5-HT receptors. Within the noradrenergic system, nefazodone inhibits norepinephrine uptake minimally. Nefazodone also antagonizes alpha(1)-adrenergic receptors, producing sedation, muscle relaxation, and a variety of cardiovascular effects. Nefazodone's affinity for benzodiazepine, cholinergic, dopaminergic, histaminic, and beta or alpha(2)-adrenergic receptors is not

				significant.
165	<chem>CN1CCOC(c2ccccc2C1)c3ccccc3</chem>	NEFOPAM	is a centrally-acting but non-opioid analgesic drug of the benzoxazocine chemical class	The mechanism of action of nefopam is not well understood, although inhibition of serotonin, dopamine and noradrenaline reuptake is thought to be involved in its analgesic effects, and there may be other modes of action such as through histamine H3 receptors and glutamate.
166	<chem>CC1C(CCN1Cc2ccccc2)NC(=O)c3cc(c(cc3OC)NC)Cl</chem>	NEMONAPRIDE	a typical antipsychotic approved in Japan for the treatment of schizophrenia	Nemonapride acts as a D ₂ and D ₃ receptor antagonist
167	<chem>CN1CCCC1c2cccnc2</chem>	NICOTINE	For the relief of nicotine withdrawal symptoms and as an aid to smoking cessation	Nicotine is a stimulant drug that acts as an agonist at nicotinic acetylcholine receptors. These are ionotropic receptors composed up of five homomeric or heteromeric subunits. In the brain, nicotine binds to nicotinic acetylcholine receptors on dopaminergic neurons in the cortico-limbic pathways

168	<chem>CC1=C(C(C(=C(N1)C)C(=O)OC(C)C)c2cccc(c2)[N+](=O)[O-])C(=O)OCCOC</chem>	NIMODIPINE	For use as an adjunct to improve neurologic outcome following subarachnoid hemorrhage (SAH) from ruptured intracranial berry aneurysms by reducing the incidence and severity of ischemic deficits	nimodipine blocks intracellular influx of calcium through voltage-dependent and receptor-operated slow calcium channels across the membranes of myocardial, vascular smooth muscle, and neuronal cells
169	<chem>c1ccc(cc1)C2=NCC(=O)Nc3c2cc(cc3)[N+](=O)[O-]</chem>	NITRAZEPAM	Used to treat short-term sleeping problems (insomnia), such as difficulty falling asleep, frequent awakenings during the night, and early-morning awakening	acts on benzodiazepine receptors in the brain which are associated with the GABA receptors
170	<chem>CCN(CC)Cc1nccn1c2c cc(cc2C(=O)c3ccccc3C l)[N+](=O)[O-]</chem>	NIZOFENONE	might thus be useful in the treatment of acute neurological conditions such as stroke	It has been shown to have neuroprotective effects and protects neurons from death following cerebral anoxia
171	<chem>CNCCC=C1c2ccccc2C Cc3c1cccc3</chem>	NORTRIPTYLINE	For the treatment of depression	either inhibits the reuptake of the neurotransmitter serotonin at the neuronal membrane or acts at beta-adrenergic receptors
172	<chem>Cc1cc2c(s1)Nc3ccccc3 N=C2N4CCN(CC4)C</chem>	OLANZAPINE	For the acute and maintenance treatment of schizophrenia and related psychotic disorders, as well as acute treatment of manic or mixed episodes of bipolar 1 disorder	likely due to a combination of antagonism at D2 receptors in the mesolimbic pathway and 5HT2A receptors in the frontal cortex

173	<chem>Cc1nccn1CC2CCc3c(c4ccccc4n3C)C2=O</chem>	ONDANSETRON	For the prevention of nausea and vomiting associated with emetogenic cancer chemotherapy	Ondansetron is a selective serotonin 5-HT ₃ receptor antagonist. The antiemetic activity of the drug is brought about through the inhibition of 5-HT ₃ receptors present both centrally (medullary chemoreceptor zone) and peripherally (GI tract)
174	<chem>Cc1ccccc1C(c2ccccc2)OCCN(C)C</chem>	ORPHENADRINE	Indicated for the treatment of Parkinson's disease.	Orphenadrine binds and inhibits both histamine H1 receptors and NMDA receptors. Orphenadrine is an anticholinergic with a predominantly central effect and only a weak peripheral effect.
175	<chem>c1ccc(cc1)C2=NC(C(=O)Nc3c2cc(cc3)Cl)O</chem>	OXAZEPAM	For the treatment of anxiety disorders and alcohol withdrawal	Similar to other benzodiazepines, oxazepam exerts its anxiolytic effects by potentiating the effect of gamma-aminobutyric acid (GABA) on GABA-A receptors through a cooperative mechanism of action. GABA receptors are ionotropic chloride-linked channel receptors that produce inhibitory postsynaptic potentials
176	<chem>c1ccc2c(c1)CC(=O)c3ccccc3N2C(=O)N</chem>	OXCARBAZEPINE	For use as monotherapy or adjunctive therapy in the treatment of partial seizures in adults with epilepsy and as adjunctive therapy in the treatment of partial seizures in children ages 4-16 with epilepsy	It is known that the pharmacological activity of oxcarbazepine occurs primarily through its 10-monohydroxy metabolite (MHD). In vitro studies indicate an MHD-induced blockade of voltage-sensitive sodium channels, resulting in stabilization of hyperexcited neuronal membranes, inhibition of repetitive neuronal discharges, and diminution of propagation of synaptic impulses

177	<chem>C1C(CN(C1=O)CC(=O)N)O</chem>	OXIRACETAM	Oxiracetam is a nootropic (memory enhancer) drug of the racetam family	oxiracetam; Belongs to the class of other agents used as CNS stimulant.
178	<chem>CN1CCC23c4c5ccc(c4OC2C(=O)CCC3(C1C5)O)OC</chem>	OXYCODONE	For the treatment of diarrhoea, pulmonary oedema and for the relief of moderate to moderately severe pain	Oxycodone acts as a weak agonist at mu, kappa, and delta opioid receptors within the central nervous system (CNS).
179	<chem>CN1CCC23c4c5ccc(c4OC2C(=O)CCC3(C1C5)O)O</chem>	OXYMORPHONE	For the treatment of moderate-to-severe pain	Oxymorphone interacts predominantly with the opioid mu-receptor. These mu-binding sites are discretely distributed in the human brain, with high densities in the posterior amygdala, hypothalamus, thalamus, nucleus caudatus, putamen, and certain cortical areas
180	<chem>Cc1c(c2cc(c(cc2[nH]1)OC)OC)CCN3CCN(CC3)c4ccccc4</chem>	OXYPERTINE	Oxypertine (Equipertine, Forit, Integrin, Lanturil, Lotawin, Opertil) is an antipsychotic used in the treatment of schizophrenia	oxypertine depletes catecholamines, though not serotonin, possibly underlying its neuroleptic efficacy
181	<chem>CC1OC(OC(O1)C)C</chem>	PARALDEHYDE	As a hypnotic/sedative & anti-seizure	It is a CNS depressant and was soon found to be an effective anticonvulsant, hypnotic and sedative

182	<chem>CCC1(C(=O)N(C(=O)O1)C)C</chem>	PARAMETHADIONE	Used for the control of absence (petit mal) seizures	Dione anticonvulsants such as paramethadione reduce T-type calcium currents in thalamic neurons (including thalamic relay neurons).
183	<chem>c1cc(ccc1C2CCNCC2COc3ccc4c(c3)OCO4)F</chem>	PAROXETINE	For the treatment of depression, depression accompanied by anxiety, obsessive compulsive disorder and panic attacks	Paroxetine is a potent and highly selective inhibitor of neuronal serotonin reuptake. Paroxetine likely inhibits the reuptake of serotonin at the neuronal membrane, enhances serotonergic neurotransmission by reducing turnover of the neurotransmitter, therefore it prolongs its activity at synaptic receptor sites and potentiates 5-HT in the CNS
184	<chem>c1ccc(cc1)C2C(=O)N=C(O2)N</chem>	PEMOLINE	For treatment of Attention Deficit Hyperactivity Disorder (ADHD)	Pemoline stimulates the brain, probably by affecting neurotransmitters
185	<chem>CC1C2Cc3ccc(cc3C1(CCN2CC=C(C)C)C)O</chem>	PENTAZOCINE	For the relief of moderate to severe pain.	The preponderance of evidence suggests that pentazocine antagonizes the opioid effects by competing for the same receptor sites, especially the opioid mu receptor
186	<chem>CCCC(C)C1(C(=O)NC(=O)NC1=O)CC</chem>	PENTOBARBITAL	For the short-term treatment of insomnia	Pentobarbital binds at a distinct binding site associated with a Cl ⁻ ionopore at the GABAA receptor, increasing the duration of time for which the Cl ⁻ ionopore is open. The post-synaptic inhibitory effect of GABA in the thalamus is, therefore, prolonged

187	<chem>CCCN1CC(CC2C1Cc3c[nH]c4c3c2ccc4)CSC</chem>	PERGOLIDE	Indicated as adjunctive treatment to levodopa/carbidopa in the management of the signs and symptoms of Parkinson's disease	Pergolide stimulates centrally-located dopaminergic receptors resulting in a number of pharmacologic effects. Five dopamine receptor types from two dopaminergic subfamilies have been identified
188	<chem>c1ccc2c(c1)N(c3cc(ccc3S2)C#N)CCCN4CCC(CC4)O</chem>	PERICYAZINE	For use as adjunctive medication in some psychotic patients. Propericiazine (Pericyazine) is used for the control of residual prevailing hostility, impulsiveness and aggressiveness.	Pericyazine, like other phenothiazines, is presumed to act principally in the subcortical areas, by producing what has been described as a central adrenergic blockade of the alpha adrenergic receptors as well as antagonism of the D(1) dopamine receptor.
189	<chem>c1ccc2c(c1)c(ns2)N3CCN(CC3)CCCCN4C(=O)C5CCCCC5C4=O</chem>	PEROSPIRONE	Perospirone (Lullan) is an atypical antipsychotic of the azapirone chemical class used for the treatment of schizophrenia and acute bipolar mania	Perospirone acts as a 5-HT _{1A} receptor partial agonist, 5-HT _{2A} receptor inverse agonist, and D ₂ , D ₄ , and α ₁ -adrenergic receptor antagonist
190	<chem>c1ccc2c(c1)N(c3cc(ccc3S2)Cl)CCCN4CCN(C4)CCO</chem>	PERPHENAZINE	management of the manifestations of psychotic disorders	Binds to the dopamine D1 and dopamine D2 receptors and inhibits their activity
191	<chem>c1ccc(cc1)CC(=O)NC(=O)N</chem>	PHENACEMIDE	treatment of epilepsy.	Phenacemide binds to and blocks neuronal sodium channels or voltage sensitive calcium channels

192	<chem>CC1C2Cc3ccc(cc3C1(CCN2CCc4ccccc4)C)O</chem>	PHENAZOCINE	opioid analgesic drug	analgesia and euphoria, also may include dysphoria and hallucinations at high doses, most likely due to action at κ -opioid and σ receptors
193	<chem>CC1C(OCCN1C)c2ccc(cc2</chem>	PHENDIMETRAZINE	management of exogenous obesity	act in a similar way to amphetamines in that it activates the alpha-adrenergic system
194	<chem>c1ccc(cc1)CCNN</chem>	PHENELZINE	treatment of major depressive disorder	irreversible, nonselective inhibition of MAO
195	<chem>CN1CCC2=C(C1)C(c3c2ccccc3)c4ccccc4</chem>	PHENINDAMINE	treat sneezing, runny nose, itching, watery eyes, hives, rashes, itching, and other symptoms of allergies	compete with histamine for histamine H ₁ -receptor sites on effector cells; an antihistamine and anticholinergic closely related to cyproheptadine; efficacy against some symptoms of opioid withdrawal
196	<chem>CCC1(C(=O)NC(=O)NC1=O)c2ccccc2</chem>	PHENOBARBITAL /PHENOBARBITONE	treatment of all types of seizures	acts on GABA _A receptors, increasing synaptic inhibition

197	<chem>CCOC(=O)C1(CCN(C1)CCC(c2ccccc2)O)c3ccccc3</chem>	PHENOPERIDINE	opioid used as a general anesthetic	It belongs to OPIATE agonist pharmacological group on the basis of mechanism of action and also classified in General Anesthetics and Analgesic-Narcotic pharmacological group.
198	<chem>CN1C(=O)CC(C1=O)c2ccccc2</chem>	PHENSUXIMIDE	treatment of epilepsy.	may act in inhibitory neuronal systems that are important in the generation of the three per second rhythm
199	<chem>CC(C)(Cc1ccccc1)N</chem>	PHENTERMINE	treatment and management of obesity.	stimulates neurons to release or maintain high levels of catecholamines
200	<chem>c1ccc(cc1)C2(C(=O)NC(=O)N2)c3ccccc3</chem>	PHENYTOIN	control of generalized tonic-clonic (grand mal) and complex partial (psychomotor, temporal lobe) seizures	acts on sodium channels on the neuronal cell membrane
201	<chem>c1ccc2c(c1)[nH]c(=O)n2C3CCN(CC3)CCCC(c4ccc(cc4)F)c5ccc(cc5)F</chem>	PIMOZIDE	suppression of motor and phonic tics in patients with Tourette's Disorder	primarily a function of its dopaminergic blocking activity of dopamine D2 receptor in the CNS

202	<chem>CC(=O)c1ccc2c(c1)N(c3ccccc3S2)CCCN4CC(C(C4)CCO</chem>	PIPERACETAZINE	First generation (typical) antipsychotic drug used for schizophrenia	All antipsychotic drugs tend to block D2 receptors in the dopamine pathways of the brain. Typical antipsychotics are not particularly selective and also block dopamine receptors in other pathways.
203	<chem>CN(C)S(=O)(=O)c1ccc2c(c1)N(c3ccccc3S2)CCCN4CCC(CC4)CCO</chem>	PIPOTHIAZINE	maintenance treatment of chronic non-agitated schizophrenic patients	Pipotiazine acts as an antagonist on dopaminergic-receptors (subtypes D1, D2, D3 and D4), on serotonergic-receptors (5-HT ₁ and 5-HT ₂)
204	<chem>C1CC(=O)N(C1)CC(=O)N</chem>	PIRACETAM	memory and cognitive enhancer; nootropic	Piracetam's mechanism of action, as with racetams in general, is not fully understood. The drug influences neuronal and vascular functions and influences cognitive function without acting as a sedative or stimulant.
205	<chem>CN1CCC(=C2c3ccccc3CCc4c2ccs4)CC1</chem>	PIZOTIFEN	prevention of vascular headache including migraine and cluster headache	serotonin antagonist acting mainly at the 5-HT ₁ , 5-HT _{2A} and 5HT _{2C} receptors
206	<chem>CCCNC1CCc2c(sc(n2)N)C1</chem>	PRAMIPEXOLE	idiopathic Parkinson's disease	stimulate dopamine receptors in the striatum; dopamine agonist with high relative in vitro specificity and full intrinsic activity at the D2 subfamily of dopamine receptors, binding with higher affinity to D3 than to D2 or D4 receptor subtypes

207	<chem>c1ccc(cc1)C2=NCC(=O)N(c3c2cc(cc3)Cl)CC4CC4</chem>	PRAZEPAM	treatment of anxiety disorders	stimulate GABA receptors in the ascending reticular activating system
208	<chem>CC(C)CC(CC(=O)O)CN</chem>	PREGABALIN	management of neuropathic pain	binds with high affinity to the alpha2-delta site (an auxiliary subunit of voltage-gated calcium channels) in central nervous system tissues
209	<chem>CCC1(C(=O)NCNC1=O)c2ccccc2</chem>	PRIMIDONE	antiepileptic	GABA receptor agonist
210	<chem>CN1CCN(CC1)CCCN2c3ccccc3Sc4c2cc(cc4)Cl</chem>	PROCHLORPERAZINE	antipsychotic, antianxiety	antidopaminergic effects mediated by somatodendritic autoreceptor D2 blockade
211	<chem>c1ccc(cc1)C(CCN2CC(C2)C3CCCCC3)O</chem>	PROCYCLIDINE	treatment of all forms of Parkinson's Disease	blocking central cholinergic receptors

212	<chem>CN(C)CCCN1c2ccccc2Sc3c1cccc3</chem>	PROMAZINE	treatment of moderate and severe psychomotor agitation	antagonist at types 1, 2, and 4 dopamine receptors, 5-HT receptor types 2A and 2C, muscarinic receptors 1 through 5, alpha(1)-receptors, and histamine H1-receptors
213	<chem>CC(CN1c2ccccc2Sc3c1cccc3)N(C)C</chem>	PROMETHAZINE	treatment of allergic disorders, and nausea/vomiting	relief of nausea appears to be related to central anticholinergic actions and may implicate activity on the medullary chemoreceptor trigger zone
214	<chem>CC(C)NCC(COc1cccc2c1cccc2)O</chem>	PROPRANOLOL	prophylaxis of migraine	competes with sympathomimetic neurotransmitters such as catecholamines for binding at beta(1)-adrenergic receptors
215	<chem>CNCCCC1c2ccccc2C=Cc3c1cccc3</chem>	PROTRIPTYLINE	treatment of depression and obsessive-compulsive disorders	decreases the reuptake of norepinephrine and serotonin
216	<chem>c1ccc(c(c1)C2=NCC(=S)N(c3c2cc(cc3)Cl)CC(F)(F)F)F</chem>	QUAZEPAM	treatment of insomnia	bind nonspecifically to benzodiazepine receptors, which affects muscle relaxation, anticonvulsant activity, motor coordination, and memory; benzodiazepine receptors are thought to be coupled to gamma-aminobutyric acid-A (GABAA) receptors, this enhances the effects of GABA by increasing GABA affinity for the GABA receptor

217	<chem>c1ccc2c(c1)C(=Nc3ccc(cc3S2)N4CCN(CC4)C</chem> <chem>COCCO</chem>	QUETIAPINE	treatment of schizophrenia and related psychotic disorders	combination of antagonism at D2 receptors in the mesolimbic pathway and 5HT2A receptors in the frontal cortex
218	<chem>CCCN1CC(CC2C1Cc3cccc(c3C2)O)NS(=O)(=O)N(CC)CC</chem>	QUINAGOLIDE	treatment of elevated levels of prolactin	a selective, D ₂ receptor agonist
219	<chem>CCCC(C)C1(C(=O)NC(=O)NC1=O)CC=C</chem>	QUINALBARBITONE	Short-term treatment of intractable insomnia for patients habituated to barbiturates	Secobarbital binds at a distinct binding site associated with a Cl ⁻ ionopore at the GABAA receptor
220	<chem>CCOc1cccc1OC(c2ccccc2)C3CNCCO3</chem>	REBOXETINE	treatment of clinical depression	selective inhibitor of noradrenaline reuptake
221	<chem>CCC(=O)N(c1ccccc1)C2(CCN(CC2)CCC(=O)OC)C(=O)OC</chem>	REMIFENTANIL	induction and maintenance of general anesthesia	a μ -opioid agonist

222	<chem>CCN1CCCC1CNC(=O)c2c(ccc(c2OC)Br)OC</chem>	REMOXIPRIDE	atypical antipsychotic	antagonist at the D2 dopamine receptor
223	<chem>Cc1c(c(=O)n2c(n1)CC(C2)CCN3CCC(CC3)c4c5ccc(cc5on4)F</chem>	RISPERIDONE	the treatment of schizophrenia	Blockade of dopaminergic D2 receptors in the limbic system
224	<chem>CCN(C)C(=O)Oc1ccc(c1)C(C)N(C)C</chem>	RIVASTIGMINE	treatment of mild to moderate dementia	binds reversibly with and inactivates cholinesterase; anticholinesterase activity of rivastigmine is relatively specific for brain acetylcholinesterase and butyrylcholinesterase compared with those in peripheral tissues
225	<chem>CN(C)CCc1c[nH]c2c1c(c(cc2)Cn3cncn3</chem>	RIZATRIPTAN	treatment of acute migraine	stimulation of presynaptic 5-HT1D receptors, direct inhibition of trigeminal nuclei cell excitability via 5-HT1B/1D receptor agonism in the brainstem and vasoconstriction of meningeal, dural, cerebral or pial vessels as a result of vascular 5-HT1B receptor agonism
226	<chem>CCCN(CCC)CCc1cccc2c1CC(=O)N2</chem>	ROPINIROLE	treatment of the signs and symptoms of idiopathic Parkinson's disease	binds the dopamine receptors D ₃ and D

227	<chem>CCCN1CCCCC1C(=O)Nc2c(cccc2C)C</chem>	ROPIVACAINE	obstetric anesthesia and regional anesthesia	block the generation and the conduction of nerve impulses
228	<chem>CC(Cc1ccccc1)N(C)CC#C</chem>	SELEGILINE	initial treatment of Parkinson's disease	irreversible inhibition of monoamine oxidase type B (MAO-B)
229	<chem>c1cc(ccc1n2cc(c3c2cc(c(c3)Cl)C4CCN(CC4)C CN5CCNC5=O)F</chem>	SERTINDOLE	treatment of schizophrenia	affinity for dopamine D2, serotonin 5-HT2A and 5-HT2C, and alpha1-adrenoreceptors
230	<chem>CNC1CCC(c2c1cccc2)c3ccc(c(c3)Cl)Cl</chem>	SERTRALINE	management of major depressive disorder, posttraumatic stress disorder, obsessive-compulsive disorder	selectively inhibit the reuptake of serotonin at the presynaptic membrane
231	<chem>CC(C)CC(C1(CCC1)c2ccc(cc2)Cl)N(C)C</chem>	SIBUTRAMINE	treatment of obesity	inhibition of norepinephrine (NE), serotonin (5-hydroxytryptamine, 5-HT), and to a lesser extent, dopamine reuptake at the neuronal synapse

232	<chem>CCC(=O)N(c1ccccc1)C2(CCN(CC2)CCc3cccs3)COC</chem>	SUFENTANIL	analgesic adjunct in anesthesia	synthetic opioid analgesic drug, approximately 5 to 10 times more potent than its analog, fentanyl
233	<chem>CCN1CCCC1CNC(=O)c2cc(ccc2OC)S(=O)(=O)N</chem>	SULPIRIDE	treatment of schizophrenia	acts primarily as a dopamine D2 antagonist
234	<chem>c1cc(ccc1N2CCCCS2(=O)=O)S(=O)(=O)N</chem>	SULTHIAME	drug of choice for benign focal epilepsies of childhood	inhibitor of carbonic anhydrase
235	<chem>CNS(=O)(=O)Cc1ccc2c(c1)c(c[nH]2)CCN(C)C</chem>	SUMATRIPTAN	treatment of migraine	binding to 5-HT1B and 5-HT1D receptors
236	<chem>c1ccc2c(c1)c(c3c(n2)C(CCC3)N</chem>	TACRINE	palliative treatment of mild to moderate dementia	anticholinesterase agent which reversibly binds with and inactivates cholinesterases

237	<chem>C=CCN1CCc2c(sc(n2)N)CC1</chem>	TALIPEXOLE	antiparkinsonian agent	dopamine agonist
238	<chem>CN1C(=O)CC(NC1=O)C(=O)NC(Cc2cnc[nH]2)C(=O)N3CCCC3C(=O)N</chem>	TALTIRELIN	treatment of Spinocerebellar ataxia	a thyrotropin-releasing hormone (TRH) analog
239	<chem>c1cnc(nc1)N2CCN(CC2)CCCCN3C(=O)C4C5CCC(C5)C4C3=O</chem>	TANDOSPIRONE	an anxiolytic and antidepressant	a potent and selective 5-HT _{1A} receptor partial agonist
240	<chem>CN1c2ccc(cc2C(=NC(C1=O)O)c3ccccc3)Cl</chem>	TEMAZEPAM	short-term treatment of insomnia	bind nonspecifically to benzodiazepine receptors
241	<chem>CC(C)CC1CN2CCc3cc(c(cc3C2CC1=O)OC)OC</chem>	TETRABENAZINE	symptomatic treatment of hyperkinetic movement disorder	promotes the early metabolic degradation of the neurotransmitter dopamine

242	<chem>c1ccc2c(c1)C(=O)N(C2=O)C3CCC(=O)NC3=O</chem>	THALIDOMIDE	sedative, antiemetic	<p>In animals the pharmacological action of thalidomide is not characteristic of the usual hypnotic agents since it does not produce loss of righting reflexes or respiratory depression. Central nervous system depression produced by thalidomide can be demonstrated by its effect on spontaneous motor activity, potentiation of central depressants, and antagonism of central stimulants. In contrast to the barbiturates, thalidomide produces a decrease in motor activity of mice in doses which do not alter motor coordination. Furthermore, it does not produce hyperactivity in low doses. Thalidomide antagonizes the hyperactivity induced in mice by caffeine and pipradrol but is less effective against the stimulant action of d-amphetamine.</p> <p>Thalidomide potentiates and prolongs the central nervous system effects of hexobarbital and barbital sodium. In some instances the potentiating effect of thalidomide is specific for certain drug actions. Thus, it potentiates the effect of anticonvulsants on maximal electroshock seizures but does not alter the acute toxicity of these drugs. It potentiates the central nervous system depressant action of chlorpromazine but does not alter significantly the dose of chlorpromazine which blocks the conditioned avoidance response.</p>
243	<chem>Cn1c2c(c(=O)n(c1=O)C)nc[nH]2</chem>	THEOPHYLLINE	treatment of the symptoms and reversible airflow obstruction associated with chronic asthma and other chronic lung diseases, such as emphysema and chronic bronchitis.	central nervous system stimulatory effect mainly on the medullary respiratory center

244	<chem>CCSc1ccc2c(c1)N(c3cccc3S2)CCCN4CCN(CC4)C</chem>	THIETHYLPERAZINE	treatment or relief of nausea and vomiting	antagonist at types 1, 2, and 4 dopamine receptors, 5-HT receptor types 2A and 2C, muscarinic receptors 1 through 5, alpha(1)-receptors, and histamine H1-receptors
245	<chem>CC(=O)OCCN1CCN(C1)CCCN2c3cccc3Sc4c2cc(cc4)Cl</chem>	THIOPROPAZATE	typical antipsychotic	All antipsychotic drugs tend to block D2 receptors in the dopamine pathways of the brain. Typical antipsychotics are not particularly selective and also block dopamine receptors in other pathways.
246	<chem>CN1CCN(CC1)CCCN2c3cccc3Sc4c2cc(cc4)S(=O)(=O)N(C)C</chem>	THIOPROPERAZINE	treatment of all types of acute and chronic schizophrenia	antagonism of D1, D2, D3, D4, 5-HT1 and 5-HT2, H1 and alpha1/alpha2-receptors
247	<chem>CN1CCCC1CCN2c3cccc3Sc4c2cc(cc4)SC</chem>	THIORIDAZINE	treatment of schizophrenia and generalized anxiety disorder	blocks postsynaptic mesolimbic dopaminergic D1 and D2 receptors in the brain
248	<chem>CN1CCN(CC1)CC/C=C/2\c3cccc3Sc4c2cc(cc4)S(=O)(=O)N(C)C</chem>	THIOTHIXENE	management of schizophrenia	antagonism of D1, D2, D3, D4, 5-HT1 and 5-HT2, H1 and alpha1/alpha2-receptors

249	<chem>Cc1ccsc1C(=CCCN2C CCC(C2)C(=O)O)c3c(c cs3)C</chem>	TIAGABINE	treatment of partial seizures	selective GABA reuptake inhibitor
250	<chem>CN1c2ccccc2C(c3ccc(cc3S1(=O)=O)Cl)NCC CCCC(=O)O</chem>	TIANEPTINE	antidepressant	modestly enhances the mesolimbic release of dopamine; has a protective effect against stress induced neuronal remodeling
251	<chem>CCOC(=O)C1(CCC=C C1N(C)C)c2ccccc2</chem>	TILIDINE	treatment of moderate to severe pain	synthetic opioid analgesic
252	<chem>Cc1ccc(cc1)C(=O)c2cc (c(c(c2)O)O)[N+](=O)[O-]</chem>	TOLCAPONE	adjunct to levodopa/carbidopa therapy for the symptomatic treatment of Parkinson's Disease	inhibits the enzyme catechol-O-methyl transferase
253	<chem>Cc1cccc(c1)N2CC(OC 2=O)CO</chem>	TOLOXATONE	antidepressant	selective reversible inhibitor of MAO-A

254	<chem>CC1(OC2COC3(C(C2O1)OC(O3)(C)C)COS(=O)(=O)N)C</chem>	TOPIRAMATE	anticonvulsant	augments the activity of the neurotransmitter gamma-aminobutyrate (GABA) at some subtypes of the GABA _A receptor; state-dependent sodium channel blocking action
255	<chem>CN(C)CC1CCCCC1(c2cccc(c2)OC)O</chem>	TRAMADOL	treatment of moderate to severe pain	selective, weak OP3-receptor agonists
256	<chem>c1ccc(cc1)C2CC2N</chem>	TRANLYCYPROMINE	treatment of major depressive episode without melancholia	irreversibly and nonselectively inhibits monoamine oxidase
257	<chem>c1ccn2c(c1)nn(c2=O)C</chem> <chem>CCN3CCN(CC3)c4ccc(c4)Cl</chem>	TRAZODONE	treatment of depression	binds at 5-HT ₂ receptor; blockage of serotonin reuptake by inhibiting serotonin reuptake pump at the presynaptic neuronal membrane
258	<chem>Cc1nnc2n1-c3ccc(cc3C(=NC2)c4ccccc4Cl)Cl</chem>	TRIAZOLAM	short-term treatment of insomnia	bind nonspecifically to benzodiazepine receptors BNZ ₁ , which mediates sleep, and BNZ ₂ , which affects muscle relaxation, anticonvulsant activity, motor coordination, and memory

259	<chem>CN1CCN(CC1)CCCN2c3cccc3Sc4c2cc(cc4)C(F)(F)F</chem>	TRIFLUOPERAZINE	treatment of anxiety disorders	blocks postsynaptic mesolimbic dopaminergic D1 and D2 receptors in the brain
260	<chem>CN(C)CCCN1c2cccc2Sc3c1cc(cc3)C(F)(F)F</chem>	TRIFLUPROMAZINE	management of psychoses	dopamine D1 and dopamine D2 receptor antagonist
261	<chem>CC(CN1c2cccc2Sc3c1cccc3)CN(C)C</chem>	TRIMEPRAZINE	a sedative, and an anti-emetic	Trimeprazine competes with free histamine for binding at HA-receptor sites. This antagonizes the effects of histamine on HA-receptors, leading to a reduction of the negative symptoms brought on by histamine HA-receptor binding.
262	<chem>CC1(C(=O)N(C(=O)O1)C)C</chem>	TRIMETHADIONE	control of absence (petit mal) seizures	reduce T-type calcium currents in thalamic neurons
263	<chem>CC(CN1c2cccc2CCc3c1cccc3)CN(C)C</chem>	TRIMIPRAMINE	treatment of depression	decreasing the reuptake of norepinephrine and serotonin

264	<chem>CN(C)CCN(Cc1ccccc1c2ccccc2)</chem>	TRIPLENNAMINE	symptomatic relief of hypersensitivity reactions	H1 receptor antagonist and functions as a weak serotonin reuptake inhibitor (SRI) and dopamine reuptake inhibitor
265	<chem>Cc1ccc(cc1)/C(=C/CN2CCCC2)/c3ccccc3</chem>	TRIPROLIDINE	antihistamine, it may cause drowsiness	H1 receptor antagonist
266	<chem>CN1C2CCC1CC(C2)OC(=O)c3c[nH]c4c3ccccc4</chem>	TROPISETRON	antiemetic	serotonin 5-HT ₃ receptor antagonist
267	<chem>CCCC(CCC)C(=O)O</chem>	VALPROIC ACID	treatment of simple and complex absence seizures	binds to and inhibits GABA transaminase
268	<chem>CN(C)CC(c1ccc(cc1)OC)C2(CCCCC2)O</chem>	VENLAFAXINE	antidepressant	inhibit the reuptake of both serotonin and norepinephrine

269	<chem>C=CC(CCC(=O)O)N</chem>	VIGABATRIN	antiseizure	inhibits gamma-aminobutyric acid transaminase GABA-T
270	<chem>CCOc1cccc1OCC2CNCCO2</chem>	VILOXAZINE	antidepressant	selective norepinephrine reuptake inhibitor
271	<chem>CCN(c1cccc(c1)c2ccnc3n2ccc3C#N)C(=O)C</chem>	ZALEPLON	treatment of insomnia	modulation of the GABA _B Z receptor chloride channel macromolecular complex
272	<chem>Cc1ccc(cc1)c2c(n3cc(cc3n2)C)CC(=O)N(C)C</chem>	ZOLPIDEM	short-term treatment of insomnia	modulates the alpha-subunit, known as the benzodiazepine receptor, within the GABA _A receptor chloride channel macromolecular complex
273	<chem>c1ccc2c(c1)c(n2)CS(=O)(=O)N</chem>	ZONISAMIDE	adjunctive treatment of partial seizures	binds to sodium channels and voltage sensitive calcium channels

274	<chem>CN1CCN(CC1)C(=O)OC2c3c(nccn3)C(=O)N2c4ccc(cn4)Cl</chem>	ZOPICLONE	short-term treatment of insomnia	binding on the benzodiazepine receptor complex and modulation of the GABA _B Z receptor chloride channel macromolecular complex
275	<chem>CN(C)CCOC1=Cc2ccc(cc2Sc3c1cc(cc3)Cl</chem>	ZOTEPINE	an atypical antipsychotic indicated for acute and chronic schizophrenia	antagonist activity at dopamine and serotonin receptors
276	<chem>c1ccc2c(c1)/C(=C\CCN3CCN(CC3)CCO)/c4cc(ccc4S2)Cl</chem>	ZUCLOPENTHIXOL	management of the manifestations of schizophrenia	antagonism of D1 and D2 dopamine receptors
277	<chem>CC(C)NCC(COc1ccccc1OCC=C)O</chem>	OXPRENOLOL	treatment of hypertension, angina pectoris, arrhythmias, and anxiety	competes with adrenergic neurotransmitters such as catecholamines for binding at sympathetic receptor
278	<chem>CC(=O)Nc1ccc(cc1)O</chem>	ACETAMINOPHEN/PARACETAMOL	relief of fever and minor aches and pains	Acetaminophen is thought to act primarily in the CNS, increasing the pain threshold by inhibiting both isoforms of cyclooxygenase, COX-1, COX-2, and COX-3 enzymes

279	<chem>CN(C)CCOC(c1ccccc1)c2ccc(cc2)Br</chem>	BROMODIPHENHYDRAMINE	antihistamine	ethanolamines have significant antimuscarinic activity and produce marked sedation in most patients
280	<chem>CC1C(OCCN1)c2ccccc2</chem>	PHENMETRAZINE	anorectic in the treatment of obesity	block the reuptake of norepinephrine and dopamine into the presynaptic neuron
281	<chem>CCOC(=O)C1(CCN(C1)CCc2ccc(cc2)N)c3ccccc3</chem>	ANILERIDINE	treatment and management of pain	opiate agonist
282	<chem>CN1CCC(CC1)OC(c2ccccc2)c3ccccc3</chem>	DIPHENYLPYRALINE	antihistamine; treatment of Parkinsonism	dopamine reuptake inhibitor
283	<chem>CCC(=O)c1ccc2c(c1)N(c3ccccc3S2)CCCN4CCN(CC4)CCO</chem>	CARPHENAZINE	antipsychotic	blocks postsynaptic mesolimbic dopaminergic D1 and D2 receptors in the brain

284	<chem>CC(=O)c1ccc2c(c1)Sc3ccccc3N2CCCN4CCN(CC4)CCO</chem>	ACETOPHENAZINE	antipsychotic	blocks postsynaptic mesolimbic dopaminergic D1 and D2 receptors in the brain
285	<chem>CC1CCN(CC1)CCCC(=O)c2ccc(cc2)F</chem>	MELPERONE	atypical antipsychotic	
286	<chem>CN1CCCC(C1)CC2c3ccccc3Sc4c2ccccc4</chem>	METIXENE	symptomatic treatment of parkinsonism	competitive antagonism of acetylcholine at muscarinic receptors in the corpus striatum
287	<chem>CC1(c2ccccc2C(=CCN(C)C)c3c1cccc3)C</chem>	MELITRACEN	antidepressant	
288	<chem>c1ccc2c(c1)CCc3ccccc3C2NCCCCCCC(=O)O</chem>	AMINEPTINE	antidepressant	selectively inhibits the reuptake of dopamine

289	<chem>CN1CCN=C(c2c1ccc(c2)Cl)c3ccccc3</chem>	MEDAZEPAM	anxiolytic, anticonvulsant, sedative and skeletal muscle relaxant	allosteric modulation of the GABA receptor
290	<chem>Cc1c(c(=O)n2ccsc2n1)CCN3CCC(=C(c4ccc(c4)F)c5ccc(cc5)F)CC3</chem>	RITANSERIN	treatment of many neurological disorders	a 5-HT _{2A} and 5-HT _{2C} receptor antagonist
291	<chem>c1ccc(c(c1)C2=NCC(=O)Nc3c2cc(cc3)Cl)Cl</chem>	DELORAZEPAM	anxiolytic, anticonvulsant	Benzodiazepines work by increasing the efficiency of a natural brain chemical, GABA, to decrease the excitability of neurons. This reduces the communication between neurons and, therefore, has a calming effect on many of the functions of the brain.
292	<chem>CNC1=Nc2ccc(cc2C(=[N+])(C1)[O-])c3ccccc3)Cl</chem>	CHLORDIAZEPOXIDE	management of anxiety disorders	binds to stereospecific benzodiazepine (BZD) binding sites on GABA (A) receptor complexes at several sites within the central nervous system
293	<chem>CN(C)Cc1nnc2n1-c3ccc(cc3C(=NC2)c4ccccc4)Cl</chem>	ADINAZOLAM	treatment of anxiety and status epilepticus	Adinazolam binds to peripheral-type benzodiazepine receptors which interact allosterically with GABA receptors. This potentiates the effects of the inhibitory neurotransmitter GABA, increasing the inhibition of the ascending reticular activating system and blocking the cortical and limbic arousal that occurs following stimulation of the reticular pathways

294	<chem>CN1CCN(CC1)C2=Nc3cccc3Sc4c2cc(cc4)Cl</chem>	CLOTHIAPINE	atypical antipsychotic	Clothiapine is a competitive antagonist to serotonin and a noncompetitive antagonist to norepinephrine, dopamine and histamine; it inhibited potassium-induced contractions in isolated rat uterus and vas deferens.
295	<chem>c1cc(ccc1C(CCCN2CC(C(CC2)(c3ccc(c(c3)C(F)(F)F)Cl)O)c4ccc(cc4)F)F</chem>	PENFLURIDOL	antipsychotic	Penfluridol blocks the postsynaptic dopamine receptor in the mesolimbic dopaminergic system and inhibits the release of hypothalamic and hypophyseal hormones
296	<chem>CN1CCC23CCCCC2C1Cc4c3cc(cc4)OC</chem>	DEXTROMETHORPHAN	treatment and relief of dry cough	antagonist to the NMDA glutamatergic receptor; agonist to the opioid sigma 1 and sigma 2 receptors, it is also an alpha3/beta4 nicotinic receptor antagonist and targets the serotonin reuptake pump
297	<chem>CCc1cc2c(s1)-n3c(nnc3CN=C2c4cccc(c4)Cl)C</chem>	ETIZOLAM	amnesic, anxiolytic, anticonvulsant, hypnotic, sedative and skeletal muscle relaxant	acts at the benzodiazepine receptors
298	<chem>CCc1cc2c(s1)N(C(=O)CN=C2c3cccc(c3)Cl)C</chem>	CLOTIAZEPAM	treatment of anxiety disorders	acts at the benzodiazepine receptors

299	<chem>CN1c2ccc(cc2C(NCC1=O)C3=CCCCC3)Cl</chem>	TETRAZEPAM	anticonvulsant, anxiolytic, hypnotic and muscle relaxant	benzodiazepine site agonist
300	<chem>c1ccc2c(c1)C=Cc3cccc(c3N2CCCN4CCN(CC4)CCO</chem>	OPIPRAMOL	antidepressant	; low to moderate affinity antagonist for the D2, 5-HT ₂ , H ₁ , H ₂ , and muscarinic acetylcholine receptors
301	<chem>CN(C)CCc1c[nH]c2c1c(c(cc2)CS(=O)(=O)N3CCCC3</chem>	ALMOTRIPTAN	treatment of acute migraine headache in adults	Almotriptan binds with high affinity to human 5-HT _{1B} and 5-HT _{1D} receptors leading to cranial blood vessel constriction
302	<chem>CCCN(CCC)C(=O)Cc1c(nc2n1cc(cc2)Cl)c3cc(c(cc3)Cl</chem>	ALPIDEM	an anxiolytic drug, approved in France in 1991 and withdrawn in 1994.	Alpidem was known to act selectively on the α_3 receptor subtype and to a lesser extent at the α_1 subtype (K_d of 0.33nM and 1.67nM respectively), of the benzodiazepine receptor. However the chemical structure of alpidem is not related to that of the benzodiazepines, and alpidem is thus sometimes referred to as a nonbenzodiazepine
303	<chem>COC(=O)C1C2CCC(N2CCCF)CC1c3ccc(cc3)I</chem>	IOFLUPANE	DaTSCAN is a solution of ioflupane (¹²³ I) for injection into a living test subject	loflupane has a high binding affinity for presynaptic dopamine transporters (DAT) in the brains of mammals, in particular the striatal region of the brain

304	<chem>CCOC(=O)c1c2n(cn1)-c3cccc(c3C(=O)N(C2)C)I</chem>	IOMAZENIL	[¹²³ I]Iomazenil ([¹²³ I]IMZ) is a ligand displaying high affinity for central-type benzodiazepine receptors, with high brain uptake and little nonspecific binding	It is a useful marker of neuronal viability. [¹²³ I]IMZ has been successfully used as a probe for single photon emission computed tomography (SPECT) in numerous clinical studies of diseases such Alzheimer's [PubMed], epilepsy [PubMed], or cerebral ischemia [PubMed], for which alterations of benzodiazepine receptors have been reported
305	<chem>CN1CCC2=C(C1)c3ccccc3Cc4c2cccc4</chem>	SETIPTILINE	tetracyclic antidepressant (TeCA) which acts as a noradrenergic and specific serotonergic antidepressant (NaSSA).	norepinephrine reuptake inhibitor, α_2 -adrenergic receptor antagonist, and serotonin receptor antagonist, likely at the 5-HT _{2A} , 5-HT _{2C} , and/or 5-HT ₃ subtypes, as well as an H ₁ receptor inverse agonist/antihistamine
306	<chem>CN(C)CCOC1=Cc2cc(ccc2Sc3c1cccc3)Cl</chem>	ZOTEPINE	atypical antipsychotic indicated for acute and chronic schizophrenia	The antipsychotic effect of zotepine is thought to be mediated through antagonist activity at dopamine and serotonin receptors. Zotepine has a high affinity for the D ₁ and D ₂ receptors. It also affects the 5-HT _{2A} , 5-HT _{2C} , 5-HT ₆ , and 5-HT ₇ receptors. In addition, it acts as a norepinephrine reuptake inhibitor, likely contributing to its efficacy against the negative symptoms of schizophrenia
307	<chem>CCN(CC)C(=O)/C(=C/c1cc(c(c1)O)O)[N+](=O)[O-]/C#N</chem>	ENTACAPONE	adjunct to levodopa / carbidopa in the symptomatic treatment of patients with idiopathic Parkinson's Disease	is believed to be through its ability to inhibit COMT in peripheral tissues, altering the plasma pharmacokinetics of levodopa; more sustained plasma levels of levodopa result in more constant dopaminergic stimulation in the brain, leading to a greater reduction in the manifestations of parkinsonian syndrome

308	<chem>CC(C)(C)C(/C=C/c1ccc2c(c1)OCO2)O</chem>	STIRIPENTOL	an anticonvulsant drug used in the treatment of epilepsy	At clinically relevant concentrations, STP enhances central GABA transmission through a barbiturate-like effect, since it increases the duration of opening of GABA-A receptors channels in hippocampal slices
309	<chem>Cn1cc2c3c1cccc3C4(C(C(CN(C4C2)C)COC(=O)c5cc(cnc5)Br)OC</chem>	NICERGOLINE	For the treatment of senile dementia, migraines of vascular origin, transient ischemia, platelet hyper-aggregability, and macular degeneration	Nicergoline acts by inhibiting the postsynaptic alpha(1)-adrenoceptors on vascular smooth muscle. This inhibits the vasoconstrictor effect of circulating and locally released catecholamines (epinephrine and norepinephrine), resulting in peripheral vasodilation. Therefore the mechanism of Nicergoline is to increase vascular circulation in the brain, thereby enhancing the transmission of nerve signals across the nerve fibres, which secrete acetylcholine as a neural transmitter.
310	<chem>c1cc(c(c(c1)Cl)Cl)N2C(CN(CC2)CCCCOc3ccc4c(c3)NC(=O)CC4</chem>	ARIPIPRAZOLE	For the treatment of schizophrenia and related psychotic disorders	Aripiprazole's antipsychotic activity is likely due to a combination of antagonism at D2 receptors in the mesolimbic pathway and 5HT2A receptors in the frontal cortex
311	<chem>c1ccc2c(c1)c(c[nH]2)C(=O)OC3CC4CC5CC(C3)N4CC5=O</chem>	DOLASETRON	For the prevention of nausea and vomiting associated with emetogenic cancer chemotherapy, including initial and repeat courses of chemotherapy.	Dolasetron is a selective serotonin 5-HT ₃ receptor antagonist

312	<chem>CNCCC(c1cccs1)Oc2c ccc3c2cccc3</chem>	DULOXETINE	For the acute and maintenance treatment of major depressive disorder (MDD), as well as acute management of generalized anxiety disorder	Duloxetine is a potent inhibitor of neuronal serotonin and norepinephrine reuptake and a less potent inhibitor of dopamine reuptake. Duloxetine has no significant affinity for dopaminergic, adrenergic, cholinergic, histaminergic, opioid, glutamate, and GABA receptors
313	<chem>c1cc(ccc1C(=O)CCCN 2CCC(CC2)(c3ccc(cc3)Br)O)F</chem>	BROMPERIDOL	used as an antipsychotic in the treatment of schizophrenia	a potent and long-acting neuroleptic
314	<chem>CCC(/C=C/Cl)(C#C)O</chem>	ETHCHLORVYNOL	Used for short-term hypnotic therapy in the management of insomnia for periods of up to one week in duration	ethchlorvynol appears to depress the central nervous system in a manner similar to that of barbiturates
315	<chem>c1c(sc(n1)CCCl</chem>	CHLORMETHIAZOLE	Clomethiazole (also called chlormethiazole) is a sedative and hypnotic that is widely used in treating and preventing symptoms of acute alcohol withdrawal	Acts like a sedative, hypnotic, muscle relaxant and anticonvulsant. Chlormethiazole acts as a positive allosteric modulator at the barbiturate/picrotoxin site of the GABA-A receptor. It works to enhance the action of the neurotransmitter GABA at this receptor.
316	<chem>CCCCC1cc(c2c(c1)O C(C3C2C=C(CC3)C)(C)C)O</chem>	DRONABINOL	For the treatment of anorexia associated with weight loss in patients with AIDS, and nausea and vomiting associated with cancer chemotherapy in patients who have failed to respond adequately to conventional antiemetic	The mechanism of action of marinol is not completely understood. It is thought that cannabinoid receptors in neural tissues may mediate the effects of dronabinol and other cannabinoids. Animal studies with other cannabinoids suggest that marinol's antiemetic effects may be due to inhibition of the vomiting control mechanism in the medulla oblongata

			treatments	
317	<chem>c1cc2c3c(c1)C(=O)N(C3CCC2)C4CN5CCC4CC5</chem>	PALONOSETRON	For the prevention of acute and delayed nausea and vomiting associated with initial and repeat courses of moderately emetogenic cancer chemotherapy, as well as prevention of acute nausea and vomiting associated with highly emetogenic cancer chemotherapy	Palonosetron is a selective serotonin 5-HT ₃ receptor antagonist. The antiemetic activity of the drug is brought about through the inhibition of 5-HT ₃ receptors present both centrally (medullary chemoreceptor zone) and peripherally (GI tract).

Table 2. List of non-CNS oral drugs studied.	
GENERIC_NAME	Canonical_Smiles
ABACAVIR SULFATE	<chem>Nc1nc(NC2CC2)c3ncn(C4CC(CO)C=C4)c3n1</chem>
ACARBOSE	<chem>CC1OC(OC2C(O)C(O)C(OC3C(O)C(O)C(O)OC3CO)OC2CO)C(O)C(O)C1NC4C=C(CO)C(O)C(O)C4O</chem>
ACEBUTOLOL	<chem>CCCC(=O)Nc1ccc(OCC(O)CNC(C)C)c(c1)C(=O)C</chem>
ACECAINIDE	<chem>CCN(CC)CCNC(=O)c1ccc(NC(=O)C)cc1</chem>
ACECLOFENAC	<chem>OC(=O)COC(=O)Cc1ccccc1Nc2c(Cl)cccc2Cl</chem>
ACEMETACIN	<chem>COc1ccc2c(c1)c(CC(=O)OCC(=O)O)c(C)n2C(=O)c3ccc(Cl)cc3</chem>
ACENOCOUMAROL	<chem>CC(=O)CC(C1=C(O)Oc2ccccc2C1=O)c3ccc(cc3)[N+](=O)[O-]</chem>
ACETOHEXAMIDE	<chem>CC(=O)c1ccc(cc1)S(=O)(=O)NC(=O)NC2CCCCC2</chem>
ACETOHYDROXAMIC ACID	<chem>CC(=O)NO</chem>
ACETYLCYSTEINE	<chem>CC(=O)NC(CS)C(=O)O</chem>

ACETYLDIGITOXIN	<chem>CC1OC(CC(OC(=O)C)C1O)OC2C(O)CC(OC3C(O)CC(OC4CCC5(C)C(CCC6C5CCC7(C)C(CCC67O)C8=CC(=O)OC8)C4)OC3C)OC2C</chem>
ACITRETIN	<chem>COc1cc(C)c(C=CC(=CC=CC(=CC(=O)O)C)C)c(C)c1C</chem>
ADEFOVIR	<chem>Nc1ncnc2c1ncn2CCOCP(=O)(O)O</chem>
ADEFOVIR DIPIVOXIL	<chem>CC(C)(C)C(=O)OCOP(=O)(COCCn1cnc2c(N)ncnc12)OCOC(=O)C(C)(C)C</chem>
ALBENDAZOLE	<chem>CCCSc1ccc2[nH]c(NC(=O)OC)nc2c1</chem>
ALCLOFENAC	<chem>OC(=O)Cc1ccc(OCC=C)c(Cl)c1</chem>
ALENDRONATE SODIUM	<chem>NCCCC(O)(P(=O)(O)O)P(=O)(O)O</chem>
ALFACALCIDOL	<chem>CC(C)CCCC(C)C1CCC2C(=CC=C3CC(O)CC(O)C3=C)CCCC12C</chem>
ALLOPURINOL	<chem>O=C1NC=Nc2[nH]ncc12</chem>
ALMITRINE	<chem>Fc1ccc(cc1)C(N2CCN(CC2)c3nc(NCC=C)nc(NCC=C)n3)c4ccc(F)cc4</chem>
ALOSETRON	<chem>Cc1[nH]cnc1CN2CCc3c(C2=O)c4ccccc4n3C</chem>

ALPRENOLOL	<chem>CC(C)NCC(O)COc1ccccc1CC=C</chem>
ALTRETAMINE	<chem>CN(C)c1nc(nc(n1)N(C)C)N(C)C</chem>
AMBENONIUM CHLORIDE	<chem>CC[N+](CC)(CCNC(=O)C(=O)NCC[N+](CC)(CC)Cc1ccccc1Cl)Cc2ccccc2Cl</chem>
AMBROXOL	<chem>Nc1c(Br)cc(Br)cc1CNC2CCC(O)CC2</chem>
AMINOCAPROIC ACID	<chem>NCCCCC(=O)O</chem>
AMINOGLUTETHIMIDE	<chem>CCC1(CCC(=O)NC1=O)c2ccc(N)cc2</chem>
AMINOSALICYLIC ACID	<chem>Nc1ccc(C(=O)O)c(O)c1</chem>
AMIODARONE HYDROCHLORIDE	<chem>CCCCc1oc2ccccc2c1C(=O)c3cc(I)c(OCCN(CC)CC)c(I)c3</chem>
AMLODIPINE BESYLATE	<chem>CCOC(=O)C1=C(COCCN)NC(=C(C1c2ccccc2Cl)C(=O)OC)C</chem>
AMODIAQUINE	<chem>CCN(CC)Cc1cc(Nc2ccnc3cc(Cl)ccc23)ccc1O</chem>
AMOXICILLIN	<chem>CC1(C)SC2C(NC(=O)C(N)c3ccc(O)cc3)C(=O)N2C1C(=O)O</chem>

AMPHOTERICIN B	<chem>CC1OC(=O)CC(O)CC(O)CCC(O)C(O)CC(O)CC2(O)CC(O)C(C(CC(OC3OC(C)C(O)C(N)C3O)C=CC=CC=CC=CC=CC=CC(C)C(O)C1C)O2)C(=O)O</chem>
AMPICILLIN	<chem>CC1(C)SC2C(NC(=O)C(N)c3ccccc3)C(=O)N2C1C(=O)O</chem>
AMPRENAVIR	<chem>CC(C)CN(CC(O)C(Cc1ccccc1)NC(=O)OC2CCOC2)S(=O)(=O)c3ccc(N)cc3</chem>
AMTOLMETIN	<chem>COc1ccccc1OC(=O)CNC(=O)Cc2ccc(C(=O)c3ccc(C)cc3)n2C</chem>
ANAGRELIDE HYDROCHLORIDE	<chem>Clc1ccc2N=C3NC(=O)CN3Cc2c1Cl</chem>
ANASTROZOLE	<chem>CC(C)(C#N)c1cc(Cn2cncn2)cc(c1)C(C)(C)C#N</chem>
ANISINDIONE	<chem>COc1ccc(cc1)C2C(=O)c3ccccc3C2=O</chem>
ANISOTROPINE	<chem>CCCC(CCC)C(=O)OC1CC2CCC(C1)[N+]2(C)C</chem>
ANTAZOLINE	<chem>C(N(Cc1ccccc1)c2ccccc2)C3=NCCN3</chem>
ARBIDOL	<chem>CCOC(=O)c1c(CSc2ccccc2)n(C)c3cc(Br)c(O)c(CN(C)C)c13</chem>
ASCORBIC	<chem>OCC(O)C1OC(=O)C(=C1O)O</chem>

ASPARTAME	<chem>COC(=O)C(Cc1ccccc1)NC(=O)C(N)CC(=O)O</chem>
ASTEMIZOLE	<chem>COc1ccc(CCN2CCC(CC2)Nc3nc4ccccc4n3Cc5ccc(F)cc5)cc1</chem>
ATAZANAVIR	<chem>COC(=O)NC(C(=O)NC(Cc1ccccc1)C(O)CN(Cc2ccc(cc2)c3cccn3)NC(=O)C(NC(=O)OC)C(C)(C)C(C)(C)C</chem>
ATENOLOL	<chem>CC(C)NCC(O)COc1ccc(CC(=O)N)cc1</chem>
ATORVASTATIN CALCIUM	<chem>CC(C)c1c(C(=O)Nc2ccccc2)c(c3ccccc3)c(c4ccc(F)cc4)n1CCC(O)CC(O)CC(=O)O</chem>
ATOVAQUONE	<chem>OC1=C(C2CCC(CC2)c3ccc(Cl)cc3)C(=O)c4ccccc4C1=O</chem>
AZACITIDINE	<chem>NC1=NC(=O)N(C=N1)C2OC(CO)C(O)C2O</chem>
AZANIDAZOLE	<chem>Cn1c(C=Cc2ccnc(N)n2)ncc1[N+](=O)[O-]</chem>
AZARIBINE	<chem>CC(=O)OCC1OC(C(OC(=O)C)C1OC(=O)C)N2N=CC(=O)NC2=O</chem>
AZATHIOPRINE	<chem>Cn1cnc(c1Sc2ncnc3[nH]cnc23)[N+](=O)[O-]</chem>
AZITHROMYCIN DIHYDRATE	<chem>CCC1OC(=O)C(C)C(OC2CC(C)(OC)C(O)C(C)O2)C(C)C(OC3OC(C)CC(C3O)N(C)C)C(C)(O)CC(C)CN(C)C(C)C(O)C1(C)O</chem>

BACAMPICILLIN HYDROCHLORIDE	<chem>CCOC(=O)OC(C)OC(=O)C1N2C(SC1(C)C)C(NC(=O)C(N)c3ccccc3)C2=O</chem>
BALSALAZIDE	<chem>OC(=O)CCNC(=O)c1ccc(cc1)N=Nc2ccc(O)c(c2)C(=O)O</chem>
BAMIFYLLINE	<chem>CCN(CCO)CCn1c(Cc2ccccc2)nc3N(C)C(=O)N(C)C(=O)c13</chem>
BEFUNOLOL	<chem>CC(C)NCC(O)COc1cccc2cc(oc12)C(=O)C</chem>
BEMETIZIDE	<chem>CC(C1Nc2cc(Cl)c(cc2S(=O)(=O)N1)S(=O)(=O)N)c3ccccc3</chem>
BENAZEPRIL	<chem>CCOC(=O)C(CCc1ccccc1)NC2CCc3ccccc3N(CC(=O)O)C2=O</chem>
BENDROFLUMETHIAZIDE	<chem>NS(=O)(=O)c1cc2c(NC(Cc3ccccc3)NS2(=O)=O)cc1C(F)(F)F</chem>
BENFLUOREX	<chem>CC(Cc1cccc(c1)C(F)(F)F)NCCOC(=O)c2ccccc2</chem>
BENORILATE	<chem>CC(=O)Nc1ccc(OC(=O)c2ccccc2OC(=O)C)cc1</chem>
BENOXAPROFEN	<chem>CC(C(=O)O)c1ccc2oc(nc2c1)c3ccc(Cl)cc3</chem>
BENTIROMIDE	<chem>OC(=O)c1ccc(NC(=O)C(Cc2ccc(O)cc2)NC(=O)c3ccccc3)cc1</chem>

BEVANTOLOL	<chem>COc1ccc(CCNCC(O)COc2cccc(C)c2)cc1OC</chem>
BEXAROTENE	<chem>Cc1cc2c(cc1C(=C)c3ccc(cc3)C(=O)O)C(C)(C)CCC2(C)C</chem>
BEZAFIBRATE	<chem>CC(C)(Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1)C(=O)O</chem>
BICALUTAMIDE	<chem>CC(O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc2ccc(C#N)c(c2)C(F)(F)F</chem>
BISACODYL	<chem>CC(=O)Oc1ccc(cc1)C(c2ccc(OC(=O)C)cc2)c3cccn3</chem>
BISOPROLOL FUMARATE	<chem>CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1</chem>
BITHIONOL	<chem>Oc1c(Cl)cc(Cl)cc1Sc2cc(Cl)cc(Cl)c2O</chem>
BOSENTAN	<chem>COc1ccccc1Oc2c(NS(=O)(=O)c3ccc(cc3)C(C)(C)C)nc(nc2OCCO)c4ncccn4</chem>
BREQUINAR	<chem>Cc1c(C(=O)O)c2cc(F)ccc2nc1c3ccc(cc3)c4ccccc4F</chem>
BRIVUDINE	<chem>OCC1OC(CC1O)N2C=C(C=CBr)C(=O)NC2=O</chem>
BROMFENAC	<chem>Nc1c(CC(=O)O)cccc1C(=O)c2ccc(Br)cc2</chem>

BROMHEXINE	<chem>CN(Cc1cc(Br)cc(Br)c1N)C2CCCCC2</chem>
BROXATEROL	<chem>CC(C)(C)NCC(O)c1onc(Br)c1</chem>
BUDESONIDE	<chem>CCCC1OC2CC3C4CCC5=CC(=O)C=CC5(C)C4C(O)CC3(C)C2(O1)C(=O)CO</chem>
BUMETANIDE	<chem>CCCCNc1cc(cc(c1Oc2ccccc2)S(=O)(=O)N)C(=O)O</chem>
BUNAZOSIN	<chem>CCCC(=O)N1CCCN(CC1)c2nc(N)c3cc(OC)c(OC)cc3n2</chem>
BUSULFAN	<chem>CS(=O)(=O)OCCCCOS(=O)(=O)C</chem>
BUTIZIDE	<chem>CC(C)CC1Nc2cc(Cl)c(cc2S(=O)(=O)N1)S(=O)(=O)N</chem>
CALCITRIOL	<chem>CC(CCCC(C)(C)O)C1CCC2C(=CC=C3CC(O)CC(O)C3=C)CCCC12C</chem>
CALUSTERONE	<chem>CC1CC2=CC(=O)CCC2(C)C3CCC4(C)C(CCC4(C)O)C13</chem>
CANDESARTAN	<chem>CCC1(O)C(=O)OCC2=C1C=C3N(Cc4cc5ccccc5nc34)C2=O</chem>
CANDESARTAN CILEXETIL	<chem>CCOc1nc2cccc(C(=O)OC(C)OC(=O)OC3CCCCC3)c2n1Cc4ccc(cc4)c5ccccc5c6nn[nH]n6</chem>

CAPECITABINE	<chem>CCCCCOC(=O)NC1=NC(=O)N(C=C1F)C2OC(C)C(O)C2O</chem>
CAPTOPRIL	<chem>CC(CS)C(=O)N1CCCC1C(=O)O</chem>
CARBAZOCHROME	<chem>CN1CC(O)C2=CC(=NNC(=O)N)C(=O)C=C12</chem>
CARBENICILLIN INDANYL SODIUM	<chem>CC1(C)SC2C(NC(=O)C(C(=O)Oc3ccc4CCc4c3)c5ccccc5)C(=O)N2C1C(=O)O</chem>
CARBENOXOLONE	<chem>CC1(C)C(CCC2(C)C1CCC3(C)C2C(=O)C=C4C5CC(C)(CCC5(C)CCC34C)C(=O)O)OC(=O)CCC(=O)O</chem>
CARBETAPENTANE	<chem>CCN(CC)CCOCCOC(=O)C1(CCCC1)c2ccccc2</chem>
CARBIDOPA	<chem>CC(Cc1ccc(O)c(O)c1)(NN)C(=O)O</chem>
CARBIMAZOLE	<chem>CCOC(=O)N1C=CN(C)C1=S</chem>
CARBOCYSTEINE	<chem>NC(CSCC(=O)O)C(=O)O</chem>
CARTEOLOL HYDROCHLORIDE	<chem>CC(C)(C)NCC(O)COc1cccc2NC(=O)CCc12</chem>
CARVEDILOL	<chem>COc1cccc1OCCNCC(O)COc2cccc3[nH]c4cccc4c23</chem>

CEFACLOR	<chem>NC(C(=O)NC1C2SCC(=C(N2C1=O)C(=O)O)Cl)c3ccccc3</chem>
CEFDINIR	<chem>Nc1nc(cs1)C(=NO)C(=O)NC2C3SCC(=C(N3C2=O)C(=O)O)C=C</chem>
CEFDITOREN	<chem>CON=C(C(=O)NC1C2SCC(=C(N2C1=O)C(=O)O)C=Cc3scnc3C)c4csc(N)n4</chem>
CEFDITOREN PIVOXIL	<chem>CON=C(C(=O)NC1C2SCC(=C(N2C1=O)C(=O)OCOC(=O)C(C)(C)C)C=Cc3scnc3C)c4csc(N)n4</chem>
CEFETAMET	<chem>CON=C(C(=O)NC1C2SCC(=C(N2C1=O)C(=O)O)C)c3csc(N)n3</chem>
CEFIXIME	<chem>Nc1nc(cs1)C(=NOCC(=O)O)C(=O)NC2C3SCC(=C(N3C2=O)C(=O)O)C=C</chem>
CEFPODOXIME	<chem>COCC1=C(N2C(SC1)C(NC(=O)C(=NOC)c3csc(N)n3)C2=O)C(=O)O</chem>
CEFPROZIL	<chem>CC=CC1=C(N2C(SC1)C(NC(=O)C(N)c3ccc(O)cc3)C2=O)C(=O)O</chem>
CEFTIBUTEN DIHYDRATE	<chem>Nc1nc(cs1)C(=CCC(=O)O)C(=O)NC2C3SCC=C(N3C2=O)C(=O)O</chem>
CEFUROXIME AXETIL	<chem>CON=C(C(=O)NC1C2SCC(=C(N2C1=O)C(=O)OC(C)OC(=O)C)COC(=O)N)c3occc3</chem>
CELECOXIB	<chem>Cc1ccc(cc1)c2cc(nn2c3ccc(cc3)S(=O)(=O)N)C(F)(F)F</chem>

CEPHALEXIN	<chem>CC1=C(N2C(SC1)C(NC(=O)C(N)c3ccccc3)C2=O)C(=O)O</chem>
CEPHALOGLYCIN	<chem>CC(=O)OCC1=C(N2C(SC1)C(NC(=O)C(N)c3ccccc3)C2=O)C(=O)O</chem>
CEPHRADINE	<chem>CC1=C(N2C(SC1)C(NC(=O)C(N)C3=CCC=CC3)C2=O)C(=O)O</chem>
CHLORAMPHENICOL	<chem>OCC(NC(=O)C(Cl)Cl)C(O)c1ccc(cc1)[N+](=O)[O-]</chem>
CHLORAMPHENICOL PALMITATE	<chem>CCCCCCCCCCCCCCCC(=O)OCC(NC(=O)C(Cl)Cl)C(O)c1ccc(cc1)[N+](=O)[O-]</chem>
CHLOROQUINE PHOSPHATE	<chem>CCN(CC)CCCC(C)Nc1ccnc2cc(Cl)ccc12</chem>
CHLOROTHIAZIDE	<chem>NS(=O)(=O)c1cc2c(cc1Cl)N=CNS2(=O)=O</chem>
CHLOROTRIANISENE	<chem>COc1ccc(cc1)C(=C(c2ccc(OC)cc2)c3ccc(OC)cc3)Cl</chem>
CHLORPROPAMIDE	<chem>CCCNC(=O)NS(=O)(=O)c1ccc(Cl)cc1</chem>
CHOLECALCIFEROL	<chem>CC(C)CCCC(C)C1CCC2C(=CC=C3CC(O)CCC3=C)CCCC12C</chem>
CICLETANINE	<chem>Cc1ncc2C(OCc2c1O)c3ccc(Cl)cc3</chem>

CILAZAPRIL	<chem>CCOC(=O)C(CCc1ccccc1)NC2CCCN3CCCC(N3C2=O)C(=O)O</chem>
CILOSTAZOL	<chem>O=C1CCc2cc(OCCCCc3nnnn3C4CCCC4)ccc2N1</chem>
CIMETIDINE	<chem>CNC(=NCCSCc1nc[nH]c1C)NC#N</chem>
CINOXACIN	<chem>CCN1N=C(C(=O)O)C(=O)c2cc3OCOc3cc12</chem>
CIPROFIBRATE	<chem>CC(C)(Oc1ccc(cc1)C2CC2(Cl)Cl)C(=O)O</chem>
CIPROFLOXACIN	<chem>OC(=O)C1=CN(C2CC2)c3cc(N4CCNCC4)c(F)cc3C1=O</chem>
CISAPRIDE MONOHYDRATE	<chem>COC1CN(CCCOc2ccc(F)cc2)CCC1NC(=O)c3cc(Cl)c(N)cc3OC</chem>
CLARITHROMYCIN	<chem>CCC1OC(=O)C(C)C(OC2CC(C)(OC)C(O)C(C)O2)C(C)C(OC3OC(C)CC(C3O)N(C)C)C(C)(CC(C)C(=O)C(C)C(O)C1(C)O)OC</chem>
CLEBOPRIDE	<chem>COc1cc(N)c(Cl)cc1C(=O)NC2CCN(Cc3ccccc3)CC2</chem>
CLENBUTEROL	<chem>CC(C)(C)NCC(O)c1cc(Cl)c(N)c(Cl)c1</chem>
CLIDINIUM BROMIDE	<chem>C[N+]12CCC(CC1)C(C2)OC(=O)C(O)(c3ccccc3)c4ccccc4</chem>

CLOBUTINOL	<chem>CC(CN(C)C)C(C)(O)Cc1ccc(Cl)cc1</chem>
CLOFAZIMINE	<chem>CC(C)N=C1C=C2N(c3ccc(Cl)cc3)c4cccc4N=C2C=C1Nc5ccc(Cl)cc5</chem>
CLOFIBRATE	<chem>CCOC(=O)C(C)(C)Oc1ccc(Cl)cc1</chem>
CLONIXIN	<chem>Cc1c(Cl)cccc1Nc2ncccc2C(=O)O</chem>
CLOPIDOGREL BISULFATE	<chem>COC(=O)C(N1CCc2sccc2C1)c3ccccc3Cl</chem>
CLOTRIMAZOLE	<chem>Clc1cccc1C(c2cccc2)(c3ccccc3)n4ccnc4</chem>
CLOXACILLIN SODIUM	<chem>Cc1onc(c2ccccc2Cl)c1C(=O)NC3C4SC(C)(C)C(N4C3=O)C(=O)O</chem>
COLCHICINE	<chem>COC1=CC=C2C(=CC1=O)C(CCC3cc(OC)c(OC)c(OC)c23)NC(=O)C</chem>
COLISTIN SULFATE	<chem>CCC(C)CCCC(=O)NC(CCN)C(=O)NC(C(C)O)C(=O)NC(CCN)C(=O)NC1CCNC(=O)C(NC(=O)C(CCN)NC(=O)C(CCN)NC(=O)C(CC(C)C)NC(=O)C(CC(C)C)NC(=O)C(CCN)NC1=O)C(C)O</chem>
CORTISONE ACETATE	<chem>CC12CCC(=O)C=C1CCC3C4CCC(O)(C(=O)CO)C4(C)CC(=O)C23</chem>

CROMOLYN SODIUM	<chem>OC(COc1cccc2OC(=CC(=O)c12)C(=O)O)COc3cccc4OC(=CC(=O)c34)C(=O)O</chem>
CYCLACILLIN	<chem>CC1(C)SC2C(NC(=O)C3(N)CCCCC3)C(=O)N2C1C(=O)O</chem>
CYCLANDELATE	<chem>CC1CC(CC(C)(C)C1)OC(=O)C(O)c2ccccc2</chem>
CYCLOBENZAPRINE HYDROCHLORIDE	<chem>CN(C)CCC=C1C=C2C=CC=CC2=Cc3ccccc13</chem>
CYCLOFENIL	<chem>CC(=O)Oc1ccc(cc1)C(=C2CCCCC2)c3ccc(OC(=O)C)cc3</chem>
CYCLOPHOSPHAMIDE	<chem>CICCN(CCCI)P1(=O)NCCCO1</chem>
CYCLOTHIAZIDE	<chem>NS(=O)(=O)c1cc2c(NC(NS2(=O)=O)C3CC4CC3C=C4)cc1Cl</chem>
CYSTEAMINE BITARTRATE	<chem>NCCS</chem>
DANAZOL	<chem>CC12Cc3cnoc3C=C1CCC4C2CCC5(C)C4CCC5(O)C#C</chem>
DAPSONE	<chem>Nc1ccc(cc1)S(=O)(=O)c2ccc(N)cc2</chem>
DEFERIPRONE	<chem>CN1C=CC(=O)C(=C1C)O</chem>

DEHYDROCHOLIC	<chem>CC(CCC(=O)O)C1CCC2C3C(CC(=O)C12C)C4(C)CCC(=O)CC4CC3=O</chem>
DELAVIRDINE MESYLATE	<chem>CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3</chem>
DEMECLOCYCLINE HYDROCHLORIDE	<chem>CN(C)C1C2CC3C(O)c4c(Cl)ccc(O)c4C(=C3C(=O)C2(O)C(=O)C(=C(N)O)C1=O)O</chem>
DESLOMATADINE	<chem>Clc1ccc2C(=C3CCNCC3)c4ncccc4CCc2c1</chem>
DESMOPRESSIN	<chem>NC(=O)CCC1NC(=O)C(Cc2ccccc2)NC(=O)C(Cc3ccc(O)cc3)NC(=O)CCSSCC(NC(=O)C(CC(=O)N)NC1=O)C(=O)N4CCCC4C(=O)NC(CCCNC(=N)N)C(=O)NCC(=O)N</chem>
DEXPANTHENOL	<chem>CC(C)(CO)C(O)C(=O)NCCCCO</chem>
DEXRAZOXANE	<chem>CC(CN1CC(=O)NC(=O)C1)N2CC(=O)NC(=O)C2</chem>
DEXTROTHYROXINE SODIUM	<chem>NC(Cc1cc(I)c(Oc2cc(I)c(O)c(I)c2)c(I)c1)C(=O)O</chem>
DIACEREIN	<chem>CC(=O)Oc1cccc2C(=O)c3cc(cc(OC(=O)C)c3C(=O)c12)C(=O)O</chem>
DIAZOXIDE	<chem>CC1=Nc2ccc(Cl)cc2S(=O)(=O)N1</chem>

DICHLORPHENAMIDE	<chem>NS(=O)(=O)c1cc(Cl)c(Cl)c(c1)S(=O)(=O)N</chem>
DICLOXACILLIN SODIUM	<chem>Cc1onc(c1C(=O)NC2C3SC(C)(C)C(N3C2=O)C(=O)O)c4c(Cl)cccc4Cl</chem>
DICUMAROL	<chem>OC1=C(CC2=C(O)c3cccc3OC2=O)C(=O)Oc4cccc14</chem>
DICYCLOMINE HYDROCHLORIDE	<chem>CCN(CC)CCOC(=O)C1(CCCCC1)C2CCCCC2</chem>
DIDANOSINE	<chem>OCC1CCC(O1)n2cnc3C(=O)NC=Nc23</chem>
DIETHYLCARBAMAZINE CITRATE	<chem>CCN(CC)C(=O)N1CCN(C)CC1</chem>
DIETHYLSTILBESTROL DIPHOSPHATE	<chem>CCC(=C(CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
DIFLUNISAL	<chem>OC(=O)c1cc(ccc1O)c2ccc(F)cc2F</chem>
DIGOXIN	<chem>CC1OC(CC(O)C1O)OC2C(O)CC(OC3C(O)CC(OC4CCC5(C)C(CCC6C5CC(O)C7(C)C(CCC67O)C8=CC(=O)OC8)C4)OC3C)OC2C</chem>
DIHYDROTACHYSTEROL	<chem>CC(C)C(C)C=CC(C)C1CCC2C(=CC=C3CC(O)CCC3C)CCCC12C</chem>
DILOXANIDE	<chem>CN(C(=O)C(Cl)Cl)c1ccc(O)cc1</chem>

DIOSMIN	<chem>COc1ccc(cc1O)C2=CC(=O)c3c(O)cc(OC4OC(COC5OC(C)C(O)C(O)C5O)C(O)C4O)cc3O2</chem>
DIPHEMANIL METHYLSULFATE	<chem>C[N+]1(C)CCC(=C(c2ccccc2)c3ccccc3)CC1</chem>
DIPYRIDAMOLE	<chem>OCCN(CCO)c1nc(N2CCCCC2)c3nc(nc(N4CCCCC4)c3n1)N(CCO)CCO</chem>
DIPYRONE	<chem>CN(CS(=O)(=O)O)C1=C(C)N(C)N(C1=O)c2ccccc2</chem>
DIRITHROMYCIN	<chem>CCC1OC(=O)C(C)C(OC2CC(C)(OC)C(O)C(C)O2)C(C)C(OC3OC(C)CC(C3O)N(C)C)C(C)(O)CC(C)C4NC(COCCOC)OC(C4C)C1(C)O</chem>
DISOPYRAMIDE	<chem>CC(C)N(CCC(C(=O)N)(c1ccccc1)c2cccn2)C(C)C</chem>
DISTIGMINE	<chem>CN(CCCCCCN(C)C(=O)Oc1ccc[n+](C)c1)C(=O)Oc2ccc[n+](C)c2</chem>
DISULFIRAM	<chem>CCN(CC)C(=S)SSC(=S)N(CC)CC</chem>
DOFETILIDE	<chem>CN(CCOc1ccc(NS(=O)(=O)C)cc1)CCc2ccc(NS(=O)(=O)C)cc2</chem>
DOXAZOSIN MESYLATE	<chem>COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5O4</chem>
DOXOFYLLINE	<chem>CN1C(=O)N(C)c2ncn(CC3OCCO3)c2C1=O</chem>

DOXYCYCLINE	<chem>CC1C2C(O)C3C(N(C)C)C(=C(C(=O)N)C(=O)C3(O)C(=C2C(=O)c4c(O)cccc14)O)O</chem>
DRONABINOL	<chem>CCCCCc1cc(O)c2C3C=C(C)CCC3C(C)(C)Oc2c1</chem>
DROSPIRENONE	<chem>CC12CCC(=O)C=C1C3CC3C4C2CCC5(C)C4C6CC6C57CCC(=O)O7</chem>
DUTASTERIDE	<chem>CC12CCC3C(CCC4NC(=O)C=CC34C)C1CCC2C(=O)Nc5cc(ccc5C(F)(F)F)C(F)(F)F</chem>
DYDROGESTERONE	<chem>CC(=O)C1CCC2C3C=CC4=CC(=O)CCC4(C)C3CCC12C</chem>
DYPHYLLINE	<chem>CN1C(=O)N(C)c2ncn(CC(O)CO)c2C1=O</chem>
EBASTINE	<chem>CC(C)(C)c1ccc(cc1)C(=O)CCCN2CCC(CC2)OC(c3ccccc3)c4ccccc4</chem>
EDETATE CALCIUM DISODIUM	<chem>OC(=O)CN(CCN(CC(=O)O)CC(=O)O)CC(=O)O</chem>
EFAVIRENZ	<chem>FC(F)(F)C1(OC(=O)Nc2ccc(Cl)cc12)C#CC3CC3</chem>
EMEPRONIUM	<chem>CC[N+](C)(C)C(C)CC(c1ccccc1)c2ccccc2</chem>
EMTRICITABINE	<chem>NC1=NC(=O)N(C=C1F)C2CSC(CO)O2</chem>

ENALAPRIL	<chem>CCOC(=O)C(CCc1ccccc1)NC(C)C(=O)N2CCCC2C(=O)O</chem>
ENCAINIDE	<chem>COc1ccc(cc1)C(=O)Nc2ccccc2C(C)CN3CCCCC3</chem>
ENOXACIN	<chem>CCN1C=C(C(=O)O)C(=O)c2cc(F)c(nc12)N3CCNCC3</chem>
ENOXIMONE	<chem>CSc1ccc(cc1)C(=O)C2=C(C)NC(=O)N2</chem>
ENPROFYLLINE	<chem>CCCN1C(=O)NC(=O)c2[nH]cnc12</chem>
EPALRESTAT	<chem>CC(=Cc1ccccc1)C=C2SC(=S)N(CC(=O)O)C2=O</chem>
EPLERENONE	<chem>COC(=O)C1CC2=CC(=O)CCC2(C)C34OC3CC5(C)C(CCC56CCC(=O)O6)C14</chem>
EPROSARTAN MESYLATE	<chem>CCCCc1ncc(C=C(Cc2cccs2)C(=O)O)n1Cc3ccc(cc3)C(=O)O</chem>
ERGOCALCIFEROL	<chem>CC(C)C(C)C=CC(C)C1CCC2C(=CC=C3CC(O)CCC3=C)CCCC12C</chem>
ERYTHRITYL	<chem>[O-][N+](=O)OCC(O[N+](=O)[O-])C(CO[N+](=O)[O-])O[N+](=O)[O-]</chem>
ERYTHROMYCIN	<chem>CCC1OC(=O)C(C)C(OC2CC(C)(OC)C(O)C(C)O2)C(C)C(OC3OC(C)CC(C3O)N(C)C)C(C)(O)CC(C)C(=O)C(C)C(O)C1(C)O</chem>

ESTRADIOL	<chem>CC12CCC3C(CCc4cc(O)ccc34)C1CCC2O</chem>
ESTRAMUSTINE	<chem>CC12CCC3C(CCc4cc(OC(=O)N(CCCl)CCCl)ccc34)C1CCC2O</chem>
ESTROPIPATE	<chem>CC12CCC3C(CCc4cc(OS(=O)(=O)O)ccc34)C1CCC2=O</chem>
ETHACRYNIC ACID	<chem>CCC(=C)C(=O)c1ccc(OCC(=O)O)c(Cl)c1Cl</chem>
ETHINYL ESTRADIOL	<chem>CC12CCC3C(CCc4cc(O)ccc34)C1CCC2(O)C#C</chem>
ETHIONAMIDE	<chem>CCc1cc(ccn1)C(=S)N</chem>
ETHYLESTRENOL	<chem>CCC1(O)CCC2C3CCC4=CCCCC4C3CCC12C</chem>
ETIDRONATE DISODIUM	<chem>CC(O)(P(=O)(O)O)P(=O)(O)O</chem>
ETILEFRINE	<chem>CCNCC(O)c1cccc(O)c1</chem>
ETODOLAC	<chem>CCc1cccc2c3CCOC(CC)(CC(=O)O)c3[nH]c12</chem>
ETORICOXIB	<chem>Cc1ccc(cn1)c2ncc(Cl)cc2c3ccc(cc3)S(=O)(=O)C</chem>

ETOZOLIN	<chem>CCOC(=O)C=C1SC(N2CCCCC2)C(=O)N1C</chem>
ETRETINATE	<chem>CCOC(=O)C=C(C)C=CC=C(C)C=Cc1c(C)cc(OC)c(C)c1C</chem>
FAMCICLOVIR	<chem>CC(=O)OCC(CCN1cnc2cnc(N)nc12)COC(=O)C</chem>
FAMOTIDINE	<chem>NC(=Nc1nc(CSCCC(=N)NS(=O)(=O)N)cs1)N</chem>
FELBINAC	<chem>OC(=O)Cc1ccc(cc1)c2ccccc2</chem>
FELODIPINE	<chem>CCOC(=O)C1=C(C)NC(=C(C1c2cccc(Cl)c2Cl)C(=O)OC)C</chem>
FENBUFEN	<chem>OC(=O)CCC(=O)c1ccc(cc1)c2ccccc2</chem>
FENOFIBRATE	<chem>CC(C)OC(=O)C(C)(C)Oc1ccc(cc1)C(=O)c2ccc(Cl)cc2</chem>
FENOPROFEN CALCIUM	<chem>CC(C(=O)O)c1cccc(Oc2ccccc2)c1</chem>
FENOTEROL	<chem>CC(Cc1ccc(O)cc1)NCC(O)c2cc(O)cc(O)c2</chem>
FENQUIZONE	<chem>NS(=O)(=O)c1cc2C(=O)NC(Nc2cc1Cl)c3ccccc3</chem>

FINASTERIDE	<chem>CC(C)(C)NC(=O)C1CCC2C3CCC4NC(=O)C=CC4(C)C3CCC12C</chem>
FLAVOXATE	<chem>CC1=C(Oc2c(cccc2C1=O)C(=O)OCCN3CCCCC3)c4ccccc4</chem>
FLECAINIDE ACETATE	<chem>FC(F)(F)COc1ccc(OCC(F)(F)F)c(c1)C(=O)NCC2CCCCN2</chem>
FLEROXACIN	<chem>CN1CCN(CC1)c2c(F)cc3C(=O)C(=CN(CCF)c3c2F)C(=O)O</chem>
FLOCTAFENINE	<chem>OCC(O)COC(=O)c1ccccc1Nc2ccnc3c(cccc23)C(F)(F)F</chem>
FLOXACILLIN	<chem>Cc1onc(c1C(=O)NC2C3SC(C)(C)C(N3C2=O)C(=O)O)c4c(F)cccc4Cl</chem>
FLUCONAZOLE	<chem>OC(Cn1cncn1)(Cn2cncn2)c3ccc(F)cc3F</chem>
FLUCYTOSINE	<chem>NC1=NC(=O)NC=C1F</chem>
FLUDROCORTISONE ACETATE	<chem>CC12CC(O)C3(F)C(CCC4=CC(=O)CCC34C)C1CCC2(O)C(=O)CO</chem>
FLUFENAMIC	<chem>OC(=O)c1ccccc1Nc2cccc(c2)C(F)(F)F</chem>
FLUMEQUINE	<chem>CC1CCc2cc(F)cc3C(=O)C(=CN1c23)C(=O)O</chem>

FLUOCORTOLONE	<chem>CC1CC2C3CC(F)C4=CC(=O)C=CC4(C)C3C(O)CC2(C)C1C(=O)CO</chem>
FLUORESCEIN	<chem>Oc1ccc2c(Oc3cc(O)ccc3C24OC(=O)c5ccccc45)c1</chem>
FLUOXYMESTERONE	<chem>CC1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3(F)C(O)CC12C</chem>
FLUPREDNISOLONE	<chem>CC12CC(O)C3C(CC(F)C4=CC(=O)C=CC34C)C1CCC2(O)C(=O)CO</chem>
FLUTAMIDE	<chem>CC(C)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](=O)[O-]</chem>
FLUTICASONE	<chem>CCC(=O)OC1(C(C)CC2C3CC(F)C4=CC(=O)C=CC4(C)C3(F)C(O)CC12C)C(=O)SCF</chem>
FLUVASTATIN SODIUM	<chem>CC(C)n1c(C=CC(O)CC(O)CC(=O)O)c(c2ccc(F)cc2)c3ccccc13</chem>
FOLIC ACID	<chem>NC1=NC(=O)c2nc(CNc3ccc(cc3)C(=O)NC(CCC(=O)O)C(=O)O)cnc2N1</chem>
FORMESTANE	<chem>CC1CCC3C(CCC4=C(O)C(=O)CCC34C)C1CCC2=O</chem>
FORMOTEROL	<chem>COC1ccc(CC(C)NCC(O)c2ccc(O)c(NC=O)c2)cc1</chem>
FOSAMPRENAVIR	<chem>CC(C)CN(CC(OP(=O)(O)O)C(Cc1ccccc1)NC(=O)OC2CCOC2)S(=O)(=O)c3cc(N)cc3</chem>

FOSFOMYCIN TROMETHAMINE	<chem>CC1OC1P(=O)(O)O</chem>
FOSINOPRIL SODIUM	<chem>CCC(=O)OC(OP(=O)(CCCCc1ccccc1)CC(=O)N2CC(CC2C(=O)O)C3CCCCC3)C(C)C</chem>
FRAMYCETIN	<chem>NCC1OC(OC2C(O)C(OC3C(O)C(N)CC(N)C3OC4OC(CN)C(O)C(O)C4N)OC2CO)C(N)C(O)C1O</chem>
FROVATRIPTAN	<chem>CNC1CCc2[nH]c3ccc(cc3c2C1)C(=O)N</chem>
FURAZOLIDONE	<chem>[O-][N+](=O)c1oc(C=NN2CCOC2=O)cc1</chem>
FUROSEMIDE	<chem>NS(=O)(=O)c1cc(C(=O)O)c(NC2occc2)cc1Cl</chem>
FUSIDIC	<chem>CC1C(O)CCC2(C)C1CCC3(C)C2C(O)CC4C(=C(CCC=C(C)C)C(=O)O)C(CC34C)OC(=O)C</chem>
GANCICLOVIR	<chem>NC1=Nc2c(ncn2COC(CO)CO)C(=O)N1</chem>
GATIFLOXACIN	<chem>COc1c(N2CCNC(C)C2)c(F)cc3C(=O)C(=CN(C4CC4)c13)C(=O)O</chem>
GEMFIBROZIL	<chem>Cc1ccc(C)c(OCCCC(C)(C)C(=O)O)c1</chem>
GEMIFLOXACIN	<chem>CON=C1CN(CC1CN)c2nc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4</chem>

GLICLAZIDE	<chem>Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2CC3CCCC3C2</chem>
GLIMEPIRIDE	<chem>CCC1=C(C)CN(C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCC(C)CC3)C1=O</chem>
GLIPIZIDE	<chem>Cc1cnc(cn1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3</chem>
GLIQUIDONE	<chem>COc1ccc2c(c1)C(=O)N(CCc3ccc(cc3)S(=O)(=O)NC(=O)NC4CCCCC4)C(=O)C2(C)C</chem>
GLISOLAMIDE	<chem>Cc1onc(c1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3</chem>
GLISOXEPIDE	<chem>Cc1onc(c1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NN3CCCCC3</chem>
GLUCOSAMINE	<chem>NC1C(O)OC(CO)C(O)C1O</chem>
GLUTAMIC ACID	<chem>NC(CCC(=O)O)C(=O)O</chem>
GLYBURIDE	<chem>COC1ccc(Cl)cc1C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3</chem>
GLYCERIN	<chem>OCC(O)CO</chem>
GLYCOPYRROLATE	<chem>C[N+](C)CCC(C1)OC(=O)C(O)(C2CCCC2)c3ccccc3</chem>

GUANADREL SULFATE	<chem>NC(=NCC1COC2(CCCCC2)O1)N</chem>
GUANFACINE HYDROCHLORIDE	<chem>NC(=N)NC(=O)Cc1c(Cl)cccc1Cl</chem>
HALOFANTRINE HYDROCHLORIDE	<chem>CCCCN(CCCC)CCC(O)c1cc2c(Cl)cc(Cl)cc2c3cc(ccc13)C(F)(F)F</chem>
HETACILLIN	<chem>CC1(C)SC2C(N3C(=O)C(NC3(C)C)c4ccccc4)C(=O)N2C1C(=O)O</chem>
HEXOCYCLIUM METHYLSULFATE	<chem>C[N+](C)CCN(CC(O)(C2CCCCC2)c3ccccc3)CC1</chem>
HEXOPRENALINE	<chem>OC(CNCCCCCNCC(O)c1ccc(O)c(O)c1)c2ccc(O)c(O)c2</chem>
HOMATROPINE METHYLBROMIDE	<chem>[Br-].C[N+](C)C2CCC1CC(C2)OC(=O)C(O)c3ccccc3</chem>
HYDRALAZINE HYDROCHLORIDE	<chem>NNc1nncc2ccccc12</chem>
HYDROCHLOROTHIAZIDE	<chem>NS(=O)(=O)c1cc2c(NCNS2(=O)=O)cc1Cl</chem>
HYDROCORTISONE	<chem>CC12CCC(=O)C=C1CCC3C4CCC(O)(C(=O)CO)C4(C)CC(O)C23</chem>
HYDROCORTISONE CYPIONATE	<chem>CC12CCC(=O)C=C1CCC3C4CCC(O)(C(=O)COC(=O)CCC5CCCC5)C4(C)CC(O)C23</chem>

HYDROFLUMETHIAZIDE	<chem>NS(=O)(=O)c1cc2c(NCNS2(=O)=O)cc1C(F)(F)F</chem>
HYDROXYUREA	<chem>NC(=O)NO</chem>
IBANDRONATE	<chem>CCCCCN(C)CCC(O)(P(=O)(O)O)P(=O)(O)O</chem>
IDARUBICIN	<chem>CC1OC(CC(N)C1O)OC2CC(O)(Cc3c(O)c4C(=O)c5cccc5C(=O)c4c(O)c23)C(=O)C</chem>
INDAPAMIDE	<chem>CC1Cc2cccc2N1NC(=O)c3ccc(Cl)c(c3)S(=O)(=O)N</chem>
INDECAINIDE HYDROCHLORIDE	<chem>CC(C)NCCCC1(C(=O)N)c2cccc2c3cccc13</chem>
INDIGOTINDISULFONATE	<chem>OS(=O)(=O)c1ccc2NC(=C3Nc4ccc(cc4C3=O)S(=O)(=O)O)C(=O)c2c1</chem>
INDINAVIR SULFATE	<chem>CC(C)(C)NC(=O)C1CN(Cc2cccnc2)CCN1CC(O)CC(Cc3cccc3)C(=O)NC4C(O)Cc5cccc45</chem>
INDOMETACIN	<chem>COc1ccc2c(c1)c(CC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C)c(C)n2C(=O)c3ccc(Cl)cc3</chem>
INDOMETHACIN	<chem>COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)c3ccc(Cl)cc3</chem>
IOCETAMIC ACID	<chem>CC(CN(C(=O)C)c1c(l)cc(l)c(N)c1l)C(=O)O</chem>

IDOQUINOL	<chem>Oc1c(I)cc(I)c2cccnc12</chem>
IOHEXOL	<chem>CC(=O)N(CC(O)CO)c1c(I)c(C(=O)NCC(O)CO)c(I)c(C(=O)NCC(O)CO)c1I</chem>
IOPANOIC ACID	<chem>CCC(Cc1c(I)cc(I)c(N)c1I)C(=O)O</chem>
IPODATE	<chem>CN(C)C=Nc1c(I)cc(I)c(CCC(=O)O)c1I</chem>
IPRIFLAVONE	<chem>CC(C)Oc1ccc2C(=O)C(=COc2c1)c3ccccc3</chem>
IRBESARTAN	<chem>CCCCC1=NC2(CCCC2)C(=O)N1Cc3ccc(cc3)c4ccccc4c5nnn[nH]5</chem>
ISONIAZID	<chem>NNC(=O)c1ccncc1</chem>
ISOPROPAMIDE IODIDE	<chem>CC(C)[N+](C)(CCC(C(=O)N)(c1ccccc1)c2ccccc2)C(C)C</chem>
ISOPROTERENOL HYDROCHLORIDE	<chem>CC(C)NCC(O)c1ccc(O)c(O)c1</chem>
ISOSORBIDE MONONITRATE	<chem>OC1COC2C(COC12)O[N+](=O)[O-]</chem>
ISOTRETINOIN	<chem>CC(=CC=CC(=CC(=O)O)C)C=CC1=C(C)CCCC1(C)C</chem>

ISOXICAM	<chem>CN1C(=C(O)c2ccccc2S1(=O)=O)C(=O)Nc3cc(C)on3</chem>
ISOXSUPRINE	<chem>CC(COc1ccccc1)NC(C)C(O)c2ccc(O)cc2</chem>
ISRADIPINE	<chem>COC(=O)C1=C(C)NC(=C(C1c2cccc3nonc23)C(=O)OC(C)C)C</chem>
ITRACONAZOLE	<chem>CCC(C)N1N=CN(C1=O)c2ccc(cc2)N3CCN(CC3)c4ccc(OCC5COC(Cn6cncn6)(O5)c7ccc(Cl)cc7Cl)cc4</chem>
IVERMECTIN	<chem>CCC(C)C1OC2(CCC1C)CC3CC(CC=C(C)C(OC4CC(OC)C(OC5CC(OC)C(O)C(C)O5)C(C)O4)C(C)C=CC=C6COC7C(O)C(=CC(C(=O)O3)C67O)C)O2</chem>
JOSAMYCIN	<chem>COC1C(CC(=O)OC(C)CC=CC=CC(O)C(C)CC(CC=O)C1OC2OC(C)C(OC3CC(C)(OC(=O)CC(C)C)C(O)C(C)O3)C(C2O)N(C)C)OC(=O)C</chem>
KANAMYCIN SULFATE	<chem>NCC1OC(OC2C(N)CC(N)C(OC3OC(CO)C(O)C(N)C3O)C2O)C(O)C(O)C1O</chem>
KETOCONAZOLE	<chem>CC(=O)N1CCN(CC1)c2ccc(OCC3COC(Cn4ccnc4)(O3)c5ccc(Cl)cc5Cl)cc2</chem>
LACIDIPINE	<chem>CCOC(=O)C1=C(C)NC(=C(C1c2ccccc2C=CC(=O)OC(C)(C)C)C(=O)OCC)C</chem>
LACTITOL	<chem>OCC(O)C(O)C(OC1OC(CO)C(O)C(O)C1O)C(O)CO</chem>

LACTULOSE	<chem>OCC(O)C(OC1OC(CO)C(O)C(O)C1O)C(O)C(=O)CO</chem>
LAMIVUDINE	<chem>NC1=NC(=O)N(C=C1)C2CSC(CO)O2</chem>
LANSOPRAZOLE	<chem>Cc1c(OCC(F)(F)F)ccnc1CS(=O)c2nc3ccccc3[nH]2</chem>
LEFLUNOMIDE	<chem>Cc1oncc1C(=O)Nc2ccc(cc2)C(F)(F)F</chem>
LERCANIDIPINE	<chem>COC(=O)C1=C(C)NC(=C(C1c2cccc(c2)[N+](=O)[O-])C(=O)OC(C)(C)CN(C)CCC(c3ccccc3)c4ccccc4)C</chem>
LETROZOLE	<chem>N#Cc1ccc(cc1)C(c2ccc(cc2)C#N)n3cncn3</chem>
LEUCOVORIN	<chem>Nc1nc(O)c2N(C=O)C(CNc3ccc(cc3)C(=O)NC(CCC(=O)O)C(=O)O)CNc2n1</chem>
LEVAMISOLE HYDROCHLORIDE	<chem>C1CN2CC(N=C2S1)c3ccccc3</chem>
LEVOCARNITINE	<chem>C[N+](C)(C)CC(O)CC(=O)O</chem>
LEVOCETIRIZINE	<chem>OC(=O)COCCN1CCN(CC1)C(c2ccccc2)c3ccc(Cl)cc3</chem>
LEVODROPROPIZINE	<chem>OCC(O)CN1CCN(CC1)c2ccccc2</chem>

LIDOFLAZINE	<chem>Cc1cccc(C)c1NC(=O)CN2CCN(CCCC(c3ccc(F)cc3)c4ccc(F)cc4)CC2</chem>
LINCOMYCIN HYDROCHLORIDE	<chem>CCCC1CC(N(C)C1)C(=O)NC(C(C)O)C2OC(SC)C(O)C(O)C2O</chem>
LIOTHYRONINE	<chem>NC(Cc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1)C(=O)O</chem>
LISINOPRIL	<chem>NCCCCC(NC(CCc1cccc1)C(=O)O)C(=O)N2CCCC2C(=O)O</chem>
LOPERAMIDE HYDROCHLORIDE	<chem>CN(C)C(=O)C(CCN1CCC(O)(CC1)c2ccc(Cl)cc2)(c3cccc3)c4cccc4</chem>
LORCAINIDE	<chem>CC(C)N1CCC(CC1)N(C(=O)Cc2cccc2)c3ccc(Cl)cc3</chem>
LOSARTAN POTASSIUM	<chem>CCCCc1nc(Cl)c(CO)n1Cc2ccc(cc2)c3cccc3c4nnn[nH]4</chem>
LOVASTATIN	<chem>CCC(C)C(=O)OC1CC(C)C=C2C=CC(C)C(CCC3CC(O)CC(=O)O3)C12</chem>
MARIMASTAT	<chem>CNC(=O)C(NC(=O)C(CC(C)C)C(O)C(=O)NO)C(C)(C)C</chem>
MEBENDAZOLE	<chem>COC(=O)Nc1nc2cc(ccc2[nH]1)C(=O)c3cccc3</chem>
MEBEVERINE	<chem>CCN(CCCCOC(=O)c1ccc(OC)c(OC)c1)C(C)Cc2ccc(OC)cc2</chem>

MECLOFENAMATE SODIUM	<chem>Cc1ccc(Cl)c(Nc2ccccc2C(=O)O)c1Cl</chem>
MEDROXYPROGESTERONE	<chem>CC1CC2C(CCC3(C)C2CCC3(O)C(=O)C)C4(C)CCC(=O)C=C14</chem>
MEFENAMIC ACID	<chem>Cc1cccc(Nc2ccccc2C(=O)O)c1C</chem>
MEFLOQUINE	<chem>OC(C1CCCCN1)c2cc(nc3c(cccc23)C(F)(F)F)C(F)(F)F</chem>
MEGESTROL ACETATE	<chem>CC(=O)C1(O)CCC2C3C=C(C)C4=CC(=O)CCC4(C)C3CCC12C</chem>
MELOXICAM	<chem>CN1C(=C(O)c2ccccc2S1(=O)=O)C(=O)Nc3ncc(C)s3</chem>
MELPHALAN	<chem>NC(Cc1ccc(cc1)N(CCCI)CCCI)C(=O)O</chem>
MENADIOL	<chem>Cc1cc(O)c2ccccc2c1O</chem>
MENADIOL SODIUM DIPHOSPHATE	<chem>CC(=O)Oc1cc(C)c(OC(=O)C)c2ccccc12</chem>
MENATETRENONE	<chem>CC(=CCCC(=CCCC(=CCCC(=CCC1=C(C)C(=O)c2ccccc2C1=O)C)C)C)C</chem>

MEPARTRICIN	<chem>COC(=O)C1C(O)CC2(O)CC(O)CC(O)CC(O)CC(O)CC(=O)CC(O)CC(=O)OC(C(C)CCC(O)CC(=O)c3ccc(N)cc3)C(C)C=CC=CC=CC=CC=CC=CC(CC1O2)OC4OC(C)C(O)C(N)C4O</chem>
MEPENZOLATE BROMIDE	<chem>C[N+](C)CCCC(C1)OC(=O)C(O)(c2ccccc2)c3ccccc3</chem>
MERCAPTOPURINE	<chem>S=C1NC=Nc2nc[nH]c12</chem>
MESALAMINE	<chem>Nc1ccc(O)c(c1)C(=O)O</chem>
MESNA	<chem>OS(=O)(=O)CCS</chem>
METAPROTERENOL	<chem>CC(C)NCC(O)c1cc(O)cc(O)c1</chem>
METHACYCLINE HYDROCHLORIDE	<chem>CN(C)C1C2C(O)C3C(=C)c4cccc(O)c4C(=O)C3=C(O)C2(O)C(=O)C(=C1O)C(=O)N</chem>
METHANTHELINE BROMIDE	<chem>CC[N+](C)(CC)CCOC(=O)C1c2ccccc2Oc3ccccc13</chem>
METHAZOLAMIDE	<chem>CN1N=C(SC1=NC(=O)C)S(=O)(=O)N</chem>
METHIMAZOLE	<chem>CN1C=CNC1=S</chem>

METHOTREXATE SODIUM	<chem>CN(Cc1cnc2nc(N)nc(N)c2n1)c3ccc(cc3)C(=O)NC(CCC(=O)O)C(=O)O</chem>
METHOXSALEN	<chem>COc1c2OC(=O)C=Cc2cc3ccoc13</chem>
METHYLCLOTHIAZIDE	<chem>CN1C(CCl)Nc2cc(Cl)c(cc2S1(=O)=O)S(=O)(=O)N</chem>
METHYLERGONOVINE	<chem>CCC(CO)NC(=O)C1CN(C)C2Cc3c[nH]c4cccc(C2=C1)c34</chem>
METHYLTESTOSTERONE	<chem>CC1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C</chem>
METOLAZONE	<chem>CC1Nc2cc(Cl)c(cc2C(=O)N1c3cccc3C)S(=O)(=O)N</chem>
METRONIDAZOLE	<chem>Cc1ncc([N+](=O)[O-])n1CCO</chem>
METYRAPONE	<chem>CC(C)(C(=O)c1cccnc1)c2cccnc2</chem>
MIDODRINE HYDROCHLORIDE	<chem>COC1ccc(OC)c(c1)C(O)CNC(=O)CN</chem>
MIGLITOL	<chem>OCCN1CC(O)C(O)C(O)C1CO</chem>
MILTEFOSINE	<chem>CCCCCCCCCCCCCCCCOP(=O)(O)OCC[N+](C)(C)C</chem>

MINOXIDIL	<chem>NC1=CC(=NC(=N)N1O)N2CCCCC2</chem>
MITOLACTOL	<chem>OC(CBr)C(O)C(O)C(O)CBr</chem>
MITOTANE	<chem>ClC(Cl)C(c1ccc(Cl)cc1)c2ccccc2Cl</chem>
MIZORIBINE	<chem>NC(=O)c1ncn(C2OC(CO)C(O)C2O)c1O</chem>
MOEXIPRIL HYDROCHLORIDE	<chem>CCOC(=O)C(CCc1ccccc1)NC(C)C(=O)N2Cc3cc(OC)c(OC)cc3CC2C(=O)O</chem>
MORICIZINE HYDROCHLORIDE	<chem>CCOC(=O)Nc1ccc2Sc3ccccc3N(C(=O)CCN4CCOCC4)c2c1</chem>
MORNIFLUMATE	<chem>FC(F)(F)c1cccc(Nc2ncccc2C(=O)OCCN3CCOCC3)c1</chem>
MOXIFLOXACIN HYDROCHLORIDE	<chem>COc1c(N2CC3CCCNC3C2)c(F)cc4C(=O)C(=CN(C5CC5)c14)C(=O)O</chem>
MYCOPHENOLATE	<chem>COc1c(C)c2COC(=O)c2c(O)c1CC=C(C)CCC(=O)O</chem>
MYCOPHENOLATE MOFETIL	<chem>COc1c(C)c2COC(=O)c2c(O)c1CC=C(C)CCC(=O)OCCN3CCOCC3</chem>
NABUMETONE	<chem>COc1ccc2cc(CCC(=O)C)ccc2c1</chem>

NAFCILLIN SODIUM	<chem>CCOc1ccc2ccccc2c1NC(=O)C3C4SC(C)(C)C(N4C3=O)C(=O)O</chem>
NALIDIXIC ACID	<chem>CCN1C=C(C(=O)O)C(=O)c2ccc(C)nc12</chem>
NATEGLINIDE	<chem>CC(C)C1CCC(CC1)C(=O)NC(Cc2ccccc2)C(=O)O</chem>
NELFINAVIR MESYLATE	<chem>Cc1c(O)cccc1C(=O)NC(CSc2ccccc2)C(O)CN3CC4CCCCC4CC3C(=O)NC(C)(C)C</chem>
NEOSTIGMINE	<chem>CN(C)C(=O)Oc1cccc(c1)[N+](C)(C)C</chem>
NEVIRAPINE	<chem>Cc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12</chem>
NIACIN	<chem>OC(=O)c1cccnc1</chem>
NICARDIPINE HYDROCHLORIDE	<chem>COC(=O)C1=C(C)NC(=C(C1c2cccc(c2)[N+](=O)[O-]))C(=O)OCCN(C)Cc3ccccc3)C</chem>
NICLOSAMIDE	<chem>Oc1ccc(Cl)cc1C(=O)Nc2ccc(cc2Cl)[N+](=O)[O-]</chem>
NICORANDIL	<chem>[O-][N+](=O)OCCNC(=O)c1cccnc1</chem>
NIFLUMIC	<chem>OC(=O)c1cccnc1Nc2cccc(c2)C(F)(F)F</chem>

NIFURTIMOX	<chem>CC1CS(=O)(=O)CCN1N=Cc2oc(cc2)[N+](=O)[O-]</chem>
NILUTAMIDE	<chem>CC1(C)NC(=O)N(C1=O)c2ccc(c(c2)C(F)(F)F)[N+](=O)[O-]</chem>
NIMESULIDE	<chem>CS(=O)(=O)Nc1ccc(cc1Oc2ccccc2)[N+](=O)[O-]</chem>
NITAZOXANIDE	<chem>CC(=O)Oc1ccccc1C(=O)Nc2ncc(s2)[N+](=O)[O-]</chem>
NITISINONE	<chem>[O-][N+](=O)c1cc(ccc1C(=O)C2C(=O)CCCC2=O)C(F)(F)F</chem>
NITRENDIPINE	<chem>CCOC(=O)C1=C(C)NC(=C(C1c2cccc(c2)[N+](=O)[O-])C(=O)OC)C</chem>
NITROFURANTOIN	<chem>[O-][N+](=O)c1oc(C=NN2CC(=O)NC2=O)cc1</chem>
NITROGLYCERIN	<chem>[O-][N+](=O)OCC(CO[N+](=O)[O-])O[N+](=O)[O-]</chem>
NIZATIDINE	<chem>CNC(=C[N+](=O)[O-])NCCSCc1csc(CN(C)C)n1</chem>
NORETHINDRONE	<chem>CC12CCC3C(CCC4=CC(=O)CCC34)C1CCC2(O)C#C</chem>
NORFLOXACIN	<chem>CCN1C=C(C(=O)O)C(=O)c2cc(F)c(cc12)N3CCNCC3</chem>

NORGESTREL	<chem>CCC12CCC3C(CCC4=CC(=O)CCC34)C1CCC2(O)C#C</chem>
NOVOBIOCIN SODIUM	<chem>COC1C(OC(=O)N)C(O)C(OC2ccc3C(=O)C(=C(O)Oc3c2C)NC(=O)c4ccc(O)c(CC=C(C)C)c4)OC1(C)C</chem>
NYLIDRIN	<chem>CC(CCc1ccccc1)NC(C)C(O)c2ccc(O)cc2</chem>
NYSTATIN	<chem>CC1OC(=O)CC(O)CC(O)CC(O)CCC(O)C(O)CC(=O)CC(O)C(C(O)CC(OC2OC(C)C(O)C(N)C2O)C=CC=CC=CC=CCCC=CC=CC(C)C(O)C1C)C(=O)O</chem>
OLMESARTAN	<chem>CCCC1nc(c(C(=O)OCC2=C(C)OC(=O)O2)n1Cc3ccc(cc3)c4ccccc4c5nnn[nH]5)C(C)(C)O</chem>
OLMESARTAN MEDOXOMIL	<chem>CCCC1nc(c(C(=O)O)n1Cc2ccc(cc2)c3ccccc3c4nnn[nH]4)C(C)(C)O</chem>
OLSALAZINE SODIUM	<chem>OC(=O)c1cc(ccc1O)N=Nc2ccc(O)c(c2)C(=O)O</chem>
OMEPRAZOLE	<chem>COc1ccc2[nH]c(nc2c1)S(=O)Cc3ncc(C)c(OC)c3C</chem>
ORLISTAT	<chem>CCCCCCCCCCCC(C1OC(=O)C1CCCCC)OC(=O)C(CC(C)C)NC=O</chem>
OSELTAMIVIR PHOSPHATE	<chem>CCOC(=O)C1=CC(OC(CC)CC)C(NC(=O)C)C(N)C1</chem>

OTILONIUM	<chem>CCCCCCCCOc1cccc1C(=O)Nc2ccc(cc2)C(=O)OCC[N+](C)(CC)CC</chem>
OXACILLIN SODIUM	<chem>Cc1onc(c2cccc2)c1C(=O)NC3C4SC(C)(C)C(N4C3=O)C(=O)O</chem>
OXAMNIQUINE	<chem>CC(C)NCC1CCc2cc(CO)c(cc2N1)[N+](=O)[O-]</chem>
OXANDROLONE	<chem>CC1(O)CCC2C3CCC4CC(=O)OCC4(C)C3CCC12C</chem>
OXAPROZIN	<chem>OC(=O)CCc1oc(c2cccc2)c(n1)c3cccc3</chem>
OXILOFRINE	<chem>CNC(C)C(O)c1ccc(O)cc1</chem>
OXOLINIC	<chem>CCN1C=C(C(=O)O)C(=O)c2cc3OCOc3cc12</chem>
OXYBUTYNIN	<chem>CCN(CC)CC#CCOC(=O)C(O)(C1CCCCC1)c2cccc2</chem>
OXYPHENBUTAZONE	<chem>CCCCC1C(=O)N(N(C1=O)c2ccc(O)cc2)c3cccc3</chem>
OXYPHENCYCLIMINE HYDROCHLORIDE	<chem>CN1CCCN=C1COC(=O)C(O)(C2CCCCC2)c3cccc3</chem>
OXYPHENONIUM BROMIDE	<chem>CC[N+](C)(CC)CCOC(=O)C(O)(C1CCCCC1)c2cccc2</chem>

OXYTETRACYCLINE	<chem>CN(C)C1C2C(O)C3C(=C(O)C2(O)C(=O)C(=C1O)C(=O)N)C(=O)c4c(O)cccc4C3(C)O</chem>
PAMIDRONATE	<chem>NCCC(O)(P(=O)(O)O)P(=O)(O)O</chem>
PANTOPRAZOLE	<chem>COc1ccnc(CS(=O)c2nc3cc(OC(F)F)ccc3[nH]2)c1OC</chem>
PANTOTHENIC	<chem>CC(C)(CO)C(O)C(=O)NCCC(=O)O</chem>
PARAMETHASONE ACETATE	<chem>CC1CC2C3CC(F)C4=CC(=O)C=CC4(C)C3C(O)CC2(C)C1(O)C(=O)CO</chem>
PAROMOMYCIN SULFATE	<chem>NCC1OC(OC2C(O)C(OC3C(O)C(N)CC(N)C3OC4OC(CO)C(O)C(O)C4N)OC2CO)C(N)C(O)C1O</chem>
PENICILLAMINE	<chem>CC(C)(S)C(N)C(=O)O</chem>
PENICILLIN V	<chem>CC1(C)SC2C(NC(=O)COc3ccccc3)C(=O)N2C1C(=O)O</chem>
PENTAERYTHRITOL	<chem>[O-][N+](=O)OCC(CO[N+](=O)[O-])(CO[N+](=O)[O-])CO[N+](=O)[O-]</chem>
PENTOXIFYLLINE	<chem>CN1C(=O)N(CCCCC(=O)C)C(=O)c2c1ncn2C</chem>
PERFLUBRON	<chem>FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br</chem>

PERINDOPRIL ERBUMINE	<chem>CCCC(NC(C)C(=O)N1C2CCCCC2CC1C(=O)O)C(=O)OCC</chem>
PERINDOPRILAT	<chem>CCCC(NC(C)C(=O)N1C2CCCCC2CC1C(=O)O)C(=O)O</chem>
PHENAZOPYRIDINE	<chem>Nc1ccc(N=Nc2ccccc2)c(N)n1</chem>
PHENFORMIN	<chem>NC(=N)NC(=N)NCCc1ccccc1</chem>
PHENINDIONE	<chem>O=C1C(C(=O)c2ccccc12)c3ccccc3</chem>
PHENOLPHTHALEIN	<chem>Oc1ccc(cc1)C2(OC(=O)c3ccccc23)c4ccc(O)cc4</chem>
PHENOXYBENZAMINE HYDROCHLORIDE	<chem>CC(COc1ccccc1)N(CCl)Cc2ccccc2</chem>
PHENPROCOUMON	<chem>CCC(C1=C(O)Oc2ccccc2C1=O)c3ccccc3</chem>
PHENYL AMINOSALICYLATE	<chem>Nc1ccc(C(=O)Oc2ccccc2)c(O)c1</chem>
PHENYLBUTAZONE	<chem>CCCCC1C(=O)N(N(C1=O)c2ccccc2)c3ccccc3</chem>
PHYTONADIONE	<chem>CC(C)CCCC(C)CCCC(C)CCCC(=CCC1=C(C)C(=O)c2ccccc2C1=O)C</chem>

PINACIDIL	<chem>CC(NC(=NC#N)Nc1ccncc1)C(C)(C)C</chem>
PINAVERIUM	<chem>COc1cc(Br)c(C[N+]2(CCOCCC3CCC4CC3C4(C)C)CCOCC2)cc1OC</chem>
PIOGLITAZONE	<chem>CCc1ccc(CCOc2ccc(CC3SC(=O)NC3=O)cc2)nc1</chem>
PIPEMIDIC	<chem>CCN1C=C(C(=O)O)C(=O)c2cnc(nc12)N3CCNCCC3</chem>
PIPERAZINE CITRATE	<chem>C1CNCCN1</chem>
PIPOBROMAN	<chem>BrCCC(=O)N1CCN(CC1)C(=O)CCBr</chem>
PIRAZOLAC	<chem>OC(=O)Cc1nn(cc1c2ccc(Cl)cc2)c3ccc(F)cc3</chem>
PIRENZEPINE	<chem>CN1CCN(CC(=O)N2c3cccc3C(=O)Nc4ccnc24)CC1</chem>
PIRITREXIM	<chem>COC1ccc(OC)c(Cc2cnc3nc(N)nc(N)c3c2C)c1</chem>
PIRMENOL	<chem>CC1CCCC(C)N1CCCC(O)(c2ccccc2)c3ccccc3</chem>
PIROXICAM	<chem>CN1C(=C(O)c2ccccc2S1(=O)=O)C(=O)Nc3ccccc3</chem>

PIROXICAM	<chem>CN1C(=C(OC(=O)C(C)(C)C)c2ccccc2S1(=O)=O)C(=O)Nc3cccn3</chem>
PIVMECILLINAM	<chem>CC(C)(C)C(=O)OCOC(=O)C1N2C(SC1(C)C)C(N=CN3CCCCC3)C2=O</chem>
POLYTHIAZIDE	<chem>CN1C(CSCC(F)(F)F)Nc2cc(Cl)c(cc2S1(=O)=O)S(=O)(=O)N</chem>
PRALIDOXIME CHLORIDE	<chem>C[n+]1ccccc1C=NO</chem>
PRAVASTATIN SODIUM	<chem>CCC(C)C(=O)OC1CC(O)C=C2C=CC(C)C(CCC(O)CC(O)CC(=O)O)C12</chem>
PRAZOSIN	<chem>COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)c4occc4</chem>
PREDNISOLONE	<chem>CC12CC(O)C3C(CCC4=CC(=O)C=CC34C)C1CCC2(O)C(=O)CO</chem>
PRIFINIUM	<chem>CC[N+]1(CC)CCC(=C(c2ccccc2)c3ccccc3)C1C</chem>
PRIMAQUINE PHOSPHATE	<chem>COc1cc(NC(C)CCCN)c2ncccc2c1</chem>
PROBENECID	<chem>CCCN(CCC)S(=O)(=O)c1ccc(cc1)C(=O)O</chem>
PROBUCOL	<chem>CC(C)(C)c1cc(SC(C)(C)Sc2cc(c(O)c(c2)C(C)(C)C(C)(C)C)cc(c1O)C(C)(C)C</chem>

PROCAINAMIDE HYDROCHLORIDE	<chem>CCN(CC)CCNC(=O)c1ccc(N)cc1</chem>
PROCARBAZINE HYDROCHLORIDE	<chem>CNNC1ccc(cc1)C(=O)NC(C)C</chem>
PROGLUMETACIN	<chem>CCCN(CCC)C(=O)C(CCC(=O)OCCCN1CCN(CCOCC(=O)Cc2c(C)n(C(=O)c3ccc(Cl)cc3)c4ccc(OC)cc24)CC1)NC(=O)c5ccccc5</chem>
PROGLUMIDE	<chem>CCCN(CCC)C(=O)C(CCC(=O)O)NC(=O)c1ccccc1</chem>
PROPICILLIN	<chem>CCC(Oc1ccccc1)C(=O)NC2C3SC(C)(C)C(N3C2=O)C(=O)O</chem>
PROPIVERINE	<chem>CCCOC(C(=O)OC1CCN(C)CC1)(c2ccccc2)c3ccccc3</chem>
PROPYLTHIOURACIL	<chem>CCCC1=CC(=O)NC(=S)N1</chem>
PROPYPHENAZONE	<chem>CC(C)C1=C(C)N(C)N(C1=O)c2ccccc2</chem>
PROQUAZONE	<chem>CC(C)N1C(=O)N=C(c2ccccc2)c3ccc(C)cc13</chem>
PROTOKYLOL HYDROCHLORIDE	<chem>CC(Cc1ccc2OCOc2c1)NCC(O)c3ccc(O)c(O)c3</chem>
PYRANTEL	<chem>CN1CCCN=C1C=Cc2cccs2</chem>

PYRIDOSTIGMINE BROMIDE	<chem>CN(C)C(=O)Oc1ccc[n+](C)c1</chem>
PYRIMETHAMINE	<chem>CCc1nc(N)nc(N)c1c2ccc(Cl)cc2</chem>
PYRVINIUM	<chem>CN(C)c1ccc2c(ccc(C=Cc3cc(C)n(c3C)c4cccc4)[n+]2C)c1</chem>
QUINACRINE	<chem>CCN(CC)CCCC(C)Nc1c2ccc(Cl)cc2nc3ccc(OC)cc13</chem>
QUINAPRIL	<chem>CCOC(=O)C(CCc1cccc1)NC(C)C(=O)N2Cc3cccc3CC2C(=O)O</chem>
QUINESTROL	<chem>CC12CCC3C(CCc4cc(OC5CCCC5)ccc34)C1CCC2(O)C#C</chem>
QUINETHAZONE	<chem>CCC1NC(=O)c2cc(c(Cl)cc2N1)S(=O)(=O)N</chem>
RACECADOTRIL	<chem>CC(=O)SCC(Cc1cccc1)C(=O)NCC(=O)OCc2cccc2</chem>
RALOXIFENE HYDROCHLORIDE	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
RAMIPRIL	<chem>CCOC(=O)C(CCc1cccc1)NC(C)C(=O)N2C3CCCC3CC2C(=O)O</chem>
RANITIDINE BISMUTH CITRATE	<chem>CNC(=C[N+])(=O)[O-])NCCSCc1oc(CN(C)C)cc1</chem>

REBAMIPIDE	<chem>OC(=O)C(CC1=CC(=O)Nc2ccccc12)NC(=O)c3ccc(Cl)cc3</chem>
RECAINAM	<chem>CC(C)NCCCNC(=O)Nc1c(C)cccc1C</chem>
REPAGLINIDE	<chem>CCOc1cc(CC(=O)NC(CC(C)C)c2ccccc2N3CCCCC3)ccc1C(=O)O</chem>
RESCINNAMINE	<chem>COC1C(CC2CN3CCc4c([nH]c5cc(OC)ccc45)C3CC2C1C(=O)OC)OC(=O)C=Cc6cc(OC)c(OC)c(OC)c6</chem>
RIBAVIRIN	<chem>NC(=O)c1ncn(n1)C2OC(CO)C(O)C2O</chem>
RIBOFLAVIN	<chem>Cc1cc2N=C3C(=O)NC(=O)N=C3N(CC(O)C(O)C(O)CO)c2cc1C</chem>
RIFABUTIN	<chem>COC1C=COC2(C)Oc3c(C)c(O)c4C(=O)C(=C5NC6(CCN(CC(C)C)CC6)N=C5c4c3C2=O)NC(=O)C(=CC=CC(C)C(O)C(C)C(O)C(C)C(OC(=O)C)C1C)C</chem>
RIFAMPIN	<chem>COC1C=COC2(C)Oc3c(C)c(O)c4c(O)c(NC(=O)C(=CC=CC(C)C(O)C(C)C(O)C(C)C(OC(=O)C)C1C)C)c(C=NN5CCN(C)CC5)c(O)c4c3C2=O</chem>
RIFAPENTINE	<chem>COC1C=COC2(C)Oc3c(C)c(O)c4c(O)c(NC(=O)C(=CC=CC(C)C(O)C(C)C(O)C(C)C(OC(=O)C)C1C)C)c(C=NN5CCN(CC5)C6CCCC6)c(O)c4c3C2=O</chem>
RIFAXIMIN	<chem>COC1C=COC2(C)Oc3c(C)c(O)c4c(O)c(NC(=O)C(=CC=CC(C)C(O)C(C)C(O)C(C)C(OC(=O)C)C1C)C)c5c(nc6cc(C)ccn56)c4c3C2=O</chem>

RILMENIDINE	<chem>C1CN=C(NC(C2CC2)C3CC3)O1</chem>
RILUZOLE	<chem>Nc1nc2ccc(OC(F)(F)F)cc2s1</chem>
RITODRINE HYDROCHLORIDE	<chem>CC(NCCc1ccc(O)cc1)C(O)c2ccc(O)cc2</chem>
RITONAVIR	<chem>CC(C)C(NC(=O)N(C)Cc1csc(n1)C(C)C)C(=O)NC(CC(O)C(Cc2ccccc2)NC(=O)OCc3cnsc3)Cc4ccccc4</chem>
ROSARAMICIN	<chem>CCC1OC(=O)CC(O)C(C)C(OC2OC(C)CC(C2O)N(C)C)C(CC=O)CC(C)C(=O)C=CC3(C)OC3C1C</chem>
ROSIGLITAZONE MALEATE	<chem>CN(CCOc1ccc(CC2SC(=O)NC2=O)cc1)c3cccn3</chem>
ROSOXACIN	<chem>CCN1C=C(C(=O)O)C(=O)c2ccc(cc12)c3ccncc3</chem>
ROSUVASTATIN	<chem>CC(C)c1nc(nc(c2ccc(F)cc2)c1C=CC(O)CC(O)CC(=O)O)N(C)S(=O)(=O)C</chem>
ROXITHROMYCIN	<chem>CCC1OC(=O)C(C)C(OC2CC(C)(OC)C(O)C(C)O2)C(C)C(OC3OC(C)CC(C3O)N(C)C)C(C)(O)CC(C)C(=NOCOCOC)C(C)C(O)C1(C)O</chem>
SALICYLAMIDE	<chem>NC(=O)c1ccccc1O</chem>
SALSALATE	<chem>OC(=O)c1ccccc1OC(=O)c2ccccc2O</chem>

SAPROPTERIN	<chem>CC(O)C(O)C1CNC2=C(N1)C(=O)NC(=N2)N</chem>
SAQUINAVIR	<chem>CC(C)(C)NC(=O)C1CC2CCCCC2CN1CC(O)C(Cc3ccccc3)NC(=O)C(CC(=O)N)NC(=O)c4ccc5ccccc5n4</chem>
SATIGREL	<chem>COC1ccc(cc1)C(=C(CCC(=O)O)C#N)c2ccc(OC)cc2</chem>
SEMATILIDE	<chem>CCN(CC)CCNC(=O)c1ccc(NS(=O)(=O)C)cc1</chem>
SILDENAFIL CITRATE	<chem>CCCc1nn(C)c2C(=O)NC(=Nc12)c3cc(ccc3OCC)S(=O)(=O)N4CCN(C)CC4</chem>
SIMVASTATIN	<chem>CCC(C)(C)C(=O)OC1CC(C)C=C2C=CC(C)C(CCC3CC(O)CC(=O)O3)C12</chem>
SIROLIMUS	<chem>COC1CC(CC(C)C2CC(=O)C(C)C=C(C)C(O)C(OC)C(=O)C(C)CC(C)C=CC=CC=C(C)C(CC3CCC(C)C(O)(O3)C(=O)C(=O)N4CCCCC4C(=O)O2)OC)CCC1O</chem>
SODIUM PHENYLBUTYRATE	<chem>OC(=O)CCCc1ccccc1</chem>
SORBINIL	<chem>Fc1ccc2OCCC3(NC(=O)NC3=O)c2c1</chem>
SORIVUDINE	<chem>OCC1OC(C(O)C1O)N2C=C(C=CBr)C(=O)NC2=O</chem>

SOTALOL HYDROCHLORIDE	<chem>CC(C)NCC(O)c1ccc(NS(=O)(=O)C)cc1</chem>
SPARFLOXACIN	<chem>CC1CN(CC(C)N1)c2c(F)c(N)c3C(=O)C(=CN(C4CC4)c3c2F)C(=O)O</chem>
SPIRAMYCIN	<chem>COC1C(O)CC(=O)OC(C)CC=CC=CC(OC2CCC(C(C)O2)N(C)C)C(C)CC(CC=O)C1OC3OC(C)C(OC4CC(C)(O)C(O)C(C)O4)C(C3O)N(C)C</chem>
SPIRAPRIL	<chem>CCOC(=O)C(CCc1ccccc1)NC(C)C(=O)N2CC3(CC2C(=O)O)SCCS3</chem>
SPIRONOLACTONE	<chem>CC(=O)SC1CC2=CC(=O)CCC2(C)C3CCC4(C)C(CCC45CCC(=O)O5)C13</chem>
STANOZOLOL	<chem>CC1(O)CCC2C3CCC4Cc5[nH]ncc5CC4(C)C3CCC12C</chem>
STAVUDINE	<chem>CC1=CN(C2OC(CO)C=C2)C(=O)NC1=O</chem>
SUCCIMER	<chem>OC(=O)C(S)C(S)C(=O)O</chem>
SUCRALFATE	<chem>OS(=O)(=O)OCC1OC(OC2(COS(=O)(=O)O)OC(OS(=O)(=O)O)C(OS(=O)(=O)O)C2OS(=O)(=O)O)C(OS(=O)(=O)O)C(OS(=O)(=O)O)C1OS(=O)(=O)O</chem>
SULFACYTINE	<chem>CCN1C=CC(=NC1=O)NS(=O)(=O)c2ccc(N)cc2</chem>

SULFADIAZINE	<chem>Nc1ccc(cc1)S(=O)(=O)Nc2ncccn2</chem>
SULFAMETER	<chem>COc1cnc(NS(=O)(=O)c2ccc(N)cc2)nc1</chem>
SULFAMETHIZOLE	<chem>Cc1nnc(NS(=O)(=O)c2ccc(N)cc2)s1</chem>
SULFAMETHOXAZOLE	<chem>Cc1onc(NS(=O)(=O)c2ccc(N)cc2)c1</chem>
SULFAPHENAZOLE	<chem>Nc1ccc(cc1)S(=O)(=O)Nc2ccnn2c3ccccc3</chem>
SULFAPYRIDINE	<chem>Nc1ccc(cc1)S(=O)(=O)Nc2ccccn2</chem>
SULFASALAZINE	<chem>OC(=O)c1cc(ccc1O)N=Nc2ccc(cc2)S(=O)(=O)Nc3ccccn3</chem>
SULFINPYRAZONE	<chem>O=C1C(CCS(=O)c2ccccc2)C(=O)N(N1c3ccccc3)c4ccccc4</chem>
SULFISOXAZOLE	<chem>Cc1noc(NS(=O)(=O)c2ccc(N)cc2)c1C</chem>
SULFISOXAZOLE ACETYL	<chem>CC(=O)N(c1onc(C)c1C)S(=O)(=O)c2ccc(N)cc2</chem>
SULFOXONE SODIUM	<chem>OS(=O)CNc1ccc(cc1)S(=O)(=O)c2ccc(NCS(=O)O)cc2</chem>

SULINDAC	<chem>CC1=C(CC(=O)O)c2cc(F)ccc2C1=Cc3ccc(cc3)S(=O)C</chem>
SULTAMICILLIN	<chem>CC1(C)SC2C(NC(=O)C(N)c3ccccc3)C(=O)N2C1C(=O)OCOC(=O)C4N5C(CC5=O)S(=O)(=O)C4(C)C</chem>
TACROLIMUS	<chem>COC1CC(CCC1O)C=C(C)C2OC(=O)C3CCCCN3C(=O)C(=O)C4(O)OC(C(CC(C)CC(=CC(CC=C)C(=O)CC(O)C2C)C)OC)C(CC4C)OC</chem>
TADALAFIL	<chem>CN1CC(=O)N2C(Cc3c([nH]c4ccccc34)C2c5ccc6OCOc6c5)C1=O</chem>
TALINOLOL	<chem>CC(C)(C)NCC(O)COc1ccc(NC(=O)NC2CCCCC2)cc1</chem>
TAMOXIFEN	<chem>CCC(=C(c1cccc1)c2ccc(OCCN(C)C)cc2)c3cccc3</chem>
TAMSULOSIN HYDROCHLORIDE	<chem>CCOc1cccc1OCCNC(C)Cc2ccc(OC)c(c2)S(=O)(=O)N</chem>
TANDOSPIRONE	<chem>O=C1C2C3CCC(C3)C2C(=O)N1CCCCN4CCN(CC4)c5ncccn5</chem>
TEGAFUR	<chem>FC1=CN(C2CCCO2)C(=O)NC1=O</chem>
TELITHROMYCIN	<chem>CCC1OC(=O)C(C)C(=O)C(C)C(OC2OC(C)CC(C2O)N(C)C)C(C)(CC(C)C(=O)C(C)C3N(CCCCn4cnc(c4)c5cccnc5)C(=O)OC13C)OC</chem>
TELMISARTAN	<chem>CCCc1nc2c(C)cc(cc2n1Cc3ccc(cc3)c4ccccc4C(=O)O)c5nc6ccccc6n5C</chem>

TEMOZOLOMIDE	<chem>CN1N=Nc2c(ncn2C1=O)C(=O)N</chem>
TENOFOVIR	<chem>CC(Cn1cnc2c(N)ncnc12)OCP(=O)(O)O</chem>
TENOXICAM	<chem>CN1C(=C(O)c2sccc2S1(=O)=O)C(=O)Nc3ccccc3</chem>
TERAZOSIN	<chem>COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4CCCCO4</chem>
TERBUTALINE SULFATE	<chem>CC(C)(C)NCC(O)c1cc(O)cc(O)c1</chem>
TESTOLACTONE	<chem>CC12CCC3C(CCC4=CC(=O)C=CC34C)C1CCC(=O)O2</chem>
TETRACYCLINE HYDROCHLORIDE	<chem>CN(C)C1C2CC3C(=C(O)C2(O)C(=O)C(=C1O)C(=O)N)C(=O)c4c(O)cccc4C3(C)O</chem>
THIABENDAZOLE	<chem>c1ccc2[nH]c(nc2c1)c3cscn3</chem>
THIACETAZONE	<chem>CC(=O)Nc1ccc(C=NNC(=S)N)cc1</chem>
THIAMPHENICOL	<chem>CS(=O)(=O)c1ccc(cc1)C(O)C(CO)NC(=O)C(Cl)Cl</chem>
THIOGUANINE	<chem>NC1=Nc2nc[nH]c2C(=S)N1</chem>

THYMOXAMINE	<chem>CC(C)c1cc(OC(=O)C)c(C)cc1OCCN(C)C</chem>
TIAPROFENIC	<chem>CC(C(=O)O)c1ccc(s1)C(=O)c2ccccc2</chem>
TICLOPIDINE HYDROCHLORIDE	<chem>Clc1ccccc1CN2CCc3sccc3C2</chem>
TICRYNAFEN	<chem>OC(=O)COc1ccc(C(=O)c2cccs2)c(Cl)c1Cl</chem>
TILUDRONATE DISODIUM	<chem>OP(=O)(O)C(Sc1ccc(Cl)cc1)P(=O)(O)O</chem>
TIMOLOL MALEATE	<chem>CC(C)(C)NCC(O)COc1nsnc1N2CCOCC2</chem>
TINIDAZOLE	<chem>CCS(=O)(=O)CCn1c(C)ncc1[N+](=O)[O-]</chem>
TIOPRONIN	<chem>CC(S)C(=O)NCC(=O)O</chem>
TIPRANAVIR	<chem>CCCC1(CCc2ccccc2)CC(=C(C(CC)c3cccc(NS(=O)(=O)c4ccc(cn4)C(F)(F)F)c3)C(=O)O1)O</chem>
TIRAPAZAMINE	<chem>Nc1n[n+](([O-]))c2ccccc2[n+][1][O-]</chem>
TOCAINIDE HYDROCHLORIDE	<chem>CC(N)C(=O)Nc1c(C)cccc1C</chem>

TOLAZAMIDE	<chem>Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2CCCCC2</chem>
TOLBUTAMIDE	<chem>CCCCNC(=O)NS(=O)(=O)c1ccc(C)cc1</chem>
TOLMETIN SODIUM	<chem>Cc1ccc(cc1)C(=O)c2ccc(CC(=O)O)n2C</chem>
TOREMIFENE CITRATE	<chem>CN(C)CCOc1ccc(cc1)C(=C(CCCl)c2ccccc2)c3ccccc3</chem>
TORSEMIDE	<chem>CC(C)NC(=O)NS(=O)(=O)c1cnccc1Nc2cccc(C)c2</chem>
TRANDOLAPRIL	<chem>CCOC(=O)C(CCC1CCCCC1)NC(C)C(=O)N2C3CCCCC3CC2C(=O)O</chem>
TRANEXAMIC ACID	<chem>NCC1CCC(CC1)C(=O)O</chem>
TRAPIDIL	<chem>CCN(CC)c1cc(C)nc2ncnn12</chem>
TREOSULFAN	<chem>CS(=O)(=O)OCC(O)C(O)COS(=O)(=O)C</chem>
TRIAMCINOLONE	<chem>CC12CC(O)C3(F)C(CCC4=CC(=O)C=CC34C)C1CC(O)C2(O)C(=O)CO</chem>
TRIAMCINOLONE DIACETATE	<chem>CC(=O)OCC(=O)C1(O)C(CC2C3CCC4=CC(=O)C=CC4(C)C3(F)C(O)CC12C)OC(=O)C</chem>

TRIAMTERENE	<chem>Nc1nc(N)c2nc(c(N)nc2n1)c3ccccc3</chem>
TRICHLORMETHIAZIDE	<chem>NS(=O)(=O)c1cc2c(NC(NS2(=O)=O)C(Cl)Cl)cc1Cl</chem>
TRICLOFOS SODIUM	<chem>OP(=O)(O)OCC(Cl)(Cl)Cl</chem>
TRIDIHEXETHYL CHLORIDE	<chem>CC[N+](CC)(CC)CCC(O)(C1CCCCC1)c2ccccc2</chem>
TRIENTINE HYDROCHLORIDE	<chem>NCCNCCNCCN</chem>
TRILOSTANE	<chem>CC12CCC3C(CCC45OC4C(=C(CC35C)C#N)O)C1CCC2O</chem>
TRIMETHOPRIM	<chem>COc1cc(Cc2cnc(N)nc2N)cc(OC)c1OC</chem>
TRIOXSALEN	<chem>CC1=CC(=O)Oc2c(C)c3oc(C)cc3cc12</chem>
TROFOSFAMIDE	<chem>CICCN(CCCI)P1(=O)OCCCN1CCCI</chem>
TROLEANDOMYCIN	<chem>COC1CC(OC2C(C)C(OC3OC(C)CC(C3OC(=O)C)N(C)C)C(C)CC4(CO4)C(=O)C(C)C(OC(=O)C)C(C)C(C)OC(=O)C2C)OC(C)C1OC(=O)C</chem>
TROVAFLOXACIN	<chem>NC1C2CN(CC12)c3nc4N(C=C(C(=O)O)C(=O)c4cc3F)c5ccc(F)cc5F</chem>

TYROPANOATE SODIUM	<chem>CCCC(=O)Nc1c(I)cc(I)c(CC(CC)C(=O)O)c1I</chem>
URACIL MUSTARD	<chem>CICCN(CCCl)C1=CNC(=O)NC1=O</chem>
URSODIOL	<chem>CC(CCC(=O)O)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CCC12C</chem>
VALACYCLOVIR HYDROCHLORIDE	<chem>CC(C)C(N)C(=O)OCCOCn1cnc2C(=O)NC(=Nc12)N</chem>
VALGANCICLOVIR HYDROCHLORIDE	<chem>CC(C)C(N)C(=O)OCC(CO)OCn1cnc2C(=O)NC(=Nc12)N</chem>
VALSARTAN	<chem>CCCCC(=O)N(Cc1ccc(cc1)c2ccccc2c3nnn[nH]3)C(C(C)C)C(=O)O</chem>
VANCOMYCIN HYDROCHLORIDE	<chem>CNC(CC(C)C)C(=O)NC1C(O)c2ccc(Oc3cc4cc(Oc5ccc(cc5Cl)C(O)C6CC(=O)C(NC(=O)C4NC(=O)C(CC(=O)N)NC1=O)c7ccc(O)c(c7)c8c(O)cc(O)cc8C(NC6=O)C(=O)O)c3OC9OC(CO)C(O)C(O)C9OC%10CC(C)(N)C(O)C(C)O%10)c(Cl)c2</chem>
VARDENAFIL	<chem>CCCC1nc(C)c2C(=O)NC(=Nn12)c3cc(ccc3OCC)S(=O)(=O)N4CCN(CC)CC4</chem>
VINCAMINE	<chem>CCC12CCCN3CCc4c(C13)n(c5ccccc45)C(O)(C2)C(=O)OC</chem>
VITAMIN	<chem>CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2c(C)c(O)c(C)c(C)c2O1</chem>

VITAMIN A PALMITATE	<chem>CCCCCCCCCCCCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C</chem>
VOGLIBOSE	<chem>OCC(CO)NC1CC(O)(CO)C(O)C(O)C1O</chem>
VORICONAZOLE	<chem>CC(c1ncncc1F)C(O)(Cn2cncn2)c3ccc(F)cc3F</chem>
WARFARIN SODIUM	<chem>CC(=O)CC(C1=C(O)c2ccccc2OC1=O)c3ccccc3</chem>
XYLOSE	<chem>OCC(O)C(O)C(O)C=O</chem>
ZAFIRLUKAST	<chem>COc1cc(ccc1Cc2cn(C)c3ccc(NC(=O)OC4CCCC4)cc23)C(=O)NS(=O)(=O)c5ccccc5C</chem>
ZALCITABINE	<chem>NC1=NC(=O)N(C=C1)C2CCC(CO)O2</chem>
ZATEBRADINE	<chem>COc1ccc(CCN(C)CCCN2CCc3cc(OC)c(OC)cc3CC2=O)cc1OC</chem>
ZOMEPIRAC	<chem>Cc1cc(CC(=O)O)n(C)c1C(=O)c2ccc(Cl)cc2</chem>